U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-286 141

Analysis of Organic Air Pollutants in the Kanawha Valley, WV and the Shenandoah Valley, VA

Research Triangle Inst, Research Triangle Park, N.C.

Prepared for

Environmental Protection Agency, Philadelphia, PA Region III

Jun 78

PB 286 141

U.S. ENVIRONMENTAL PROTECTION AGENCY

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

MIDDLE ATLANTIC REGION-III 6th and Walnut Streets, Philadelphia, Pennsylvania 19106

EPA-903/9-78-007

ANALYSIS OF ORGANIC AIR POLLUTANTS IN THE KANAWHA VALLEY, WV AND THE SHENANDOAH VALLEY, VA

by

Mitchell D. Erickson

and

17 Edo D. Pellizzari 17

June, 1978

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-903/9-78-007	2.	3. RE 'S ACCESSION NO. PB286141
4. TITLE AND SUBTITLE ANALYSIS OF ORGANIC AIR POLLUTANTS IN THE KANAWHA VALLEY, WV AND THE SHENANDOAH VALLEY, VA		5. REPORT DATE June 1978 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Edo D. Pellizzari Mitchell D. Erickson		8. PERFORMING ORGANIZATION REPORT NO. RTI/1401/00-01F
9. PERFORMING ORGANIZATION NAME AND ADDRESS Research Triangle Institute P. O. Box 12194 Research Triangle Park, NC 27709		10. PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO. BOA 68-02-2543, Order No. 1
12. SPONSORING AGENCY NAME AND ADDRESS U. S. Environmental Protection Agency Region III 6th and Walnut Streets Philadelphia, PA 19106		13. TYPE OF REPORT AND PERIOD COVERED FINAL, Aug. 10 '77-Dec. 9 '77 14. SPONSORING AGENCY CODE 903/00

15. SUPPLEMENTARY NOTES

Project Officer is Daniel FitzGerald

16. ABSTRACT

Recently developed techniques for sampling and analysis of ambient air by GC/MS/COMP were applied to the Kanawha Valley, WV and Shenandoah Valley, VA to assess the levels of organic pollutants. Volatile and very volatile compounds were concentrated on Tenax GC and carbon sorbent cartridges, respectively, then thermally desorbed directly into the capillary column GC/MS/COMP system for analysis. Semivolatiles were collected on the electrostatic precipitator plates of a Massive Air Sampler, extracted, fractionated, and then analyzed by GC/MS/COMP. The Kanawha Valley contained a broad range of halogenated, ketone, aldehyde, ester, aromatic, aliphatic and polynuclear aromatic compounds. The Shenandoah Valley contained a narrower range of organics, but generally higher observed levels of the compounds quantitated.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
GC/MS/COMP	Air Sampling		
Air Pollution	Gas Chromatography		
Air Pollution Sampling	Mass Spectrometry		
Kanawha Valley, WV	Organic Compounds		
Shenandoah Valley, VA			
Charleston, WV			
Front Royal, VA			

18. DISTRIBUTION STATEMENT UNLIMITED	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 192
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE A09-A01

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

DISCLAIMER

This report has been reviewed by the Region III U. S. Environmental Protection Agency, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the U. S. Environmental Protection Agency, nor does mention of trade names of commercial products constitute endorsement or recommendation for use.

ABSTRACT

Recently developed techniques for sampling and analysis of ambient air by GC/MS/COMP were applied to the Kanawha Valley, WV and Shenandoah Valley, VA to assess the levels of organic pollutants. Volatile and very volatile compounds were concentrated on Tenax GC and carbon sorbent cartridges, respectively, then thermally desorbed directly into the capillary column GC/MS/COMP system for analysis. Semivolatiles were collected on the electrostatic precipitator plates of a Massive Air Sampler, extracted, fractionated, and then analyzed by GC/MS/COMP. The Kanawha Valley contained a broad range of halogenated, ketone, aldehyde, ester, aromatic, aliphatic and polynuclear aromatic compounds. The Shenandoah Valley contained a narrower range of organics, but generally higher observed levels of the compounds quantitated.

CONTENTS

Page

Abstract iii
Figures vi
Tables viii
Acknowledgements xii

1. Introduction 1
2. Summary and Conclusions 2
3. Recommendations 5
4. Objectives 7
5. Sampling 8
6. Sample Analysis 33
7. Results 38
8. Quality Control 71

References 76

Appendix

A. Sampling and Analysis for Volatile Organics in Ambient Air . 78
B. Sampling and Analysis for Very Volatile Organics (e.g., Methyl Chloride, Methyl Bromide, Vinyl Chloride and Vinyl Bromide) in Ambient Air 106
C. Volatile and Very Volatile Organic Compounds Identified in Air in the Kanawha Valley, WV 118
D. Semivolatile Compounds Identified in Air Particulate Collected in Kanawha Valley, WV 146
E. Volatile and Very Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA 156
F. Semivolatile Compounds Identified in Air Particulate Collected in Shenandoah Valley, VA 173

FIGURES

Number		Page
1	Collection system for concentrating high and medium volatility organic compounds from ambient air	9
2	The Kanawha River Valley, West Virginia	14
3	Map of area around Nitro, WV showing L4, L6, L7, and L9 (See Table 1)	20
4	Map of area around St. Albans and Institute, WV showing L3 and L8 (See Table 1).	21
5	Map of area around Charleston and South Charleston, WV showing L1 and L2 (See Table 1).	22
6	Map of area around W. Belle, WV showing L5 (See Table 1). . . .	23
7	Front Royal, VA	25
8	Map of Front Royal, VA showing locations described in Table 5	30
9	Fractionation scheme used for fractionating air particulate collected in Charleston, WV (Trip 3, P1/L1)	35
10	Extraction scheme for particulate collected in Front Royal, VA.	37
11	Field Sampling Protocol Data Sheet	72
A-1	Vapor collection and analytical systems for analysis of organic vapors in ambient air	80
A-2	Sampling head for housing cartridge sampling train	88
A-3	Profile of ambient air pollutants for Wood River, IL using high resolution gas chromatography/mass spectrometry/-computer.	95
A-4	Background profile for Tenax GC cartridge blank	96
A-5	Schematic diagram of gc-ms computer system	97
A-6	Mass fragmentograms of characteristic ions representating carbon tetrachloride (m/e 117), tetrachloroethylene (m/e 166) and m-dichlorobenzene (m/e 146) in ambient air	101

FIGURES (cont'd.)

Number Page

A-7 Mass fragmentograms of characteristic ions representating methylene chloride (m/e 49) and chloroform (m/e 83) in ambient air 102

B-1 Nutech Model 221-A AC-DC Sampler 108

D-1 Total ion current chromatogram of GC/MS/COMP analysis of polar neutral fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1). 152

D-2 Total ion current chromatogram of GC/MS/COMP analysis of PNA fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1). 153

D-3 Total ion current chromatogram of GC/MS/COMP analysis of paraffin fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1). 154

D-4 Total ion current chromatogram of GC/MS/COMP analysis of base fraction of < 1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1). 155

F-1 Total ion current chromatogram of GC/MS/COMP analysis of methanol extract of <1.7μ air particulate collected in Front Royal, VA (Trip 3, P1/L4). 174

F-2 Total ion current chromatogram of GC/MS/COMP analysis of toluene extract of <1.7μ air particulate collected in Front Royal, VA (Trip 3, P1/L4). 176

TABLES

Number Page

1 Sampling Locations in the Kanawha Valley, WV 16

2 Sampling Protocol for Organic Compounds in Ambient Air in Kanawha Valley, WV --- Trip 1 17

3 Sampling Protocol for Organic Compounds in Ambient Air in Kanawha Valley, WV --- Trip 2 18

4 Sampling Protocol for Organic Compouns in Ambient Air in Kanawha Valley, WV --- Trip 3 19

5 Sampling Locations in the Shenandoah Valley, VA 26

6 Sampling Protocol for Organic Compounds in Ambient Air in Shenandoah Valley, VA --- Trip 1 27

7 Sampling Protocol for Organic Compounds in Ambient Air in Shenandoah Valley, VA --- Trip 2 28

8 Sampling Protocol for Organic Compounds in Ambient Air in Shenandoah Valley, VA --- Trip 3 29

9 Summary of Particulate Sampling with MAS for Shenandoah and Kanawha Valleys 32

10 Recoveries of Selected Organic Vapors from Tenax Cartridges Subjected to Sample Transportation and Storage 39

11 Volatile Organics Identified in Ambient Air in the Kanawha Valley, WV 41

12 Estimated Levels of Halogenated Organic Vapors in Ambient Air from the Kanawha Valley, WV --- Trip 1 51

13 Estimated Levels of Halogenated Organic Vapors in Ambient Air from the Kanawha Valley, WV --- Trip 2 52

14 Estimated Levels of Halogenated Organic Vapors in Ambient Air from the Kanawha Valley, WV --- Trip 3 53

15 Estimated Levels of Volatile Organics in Ambient Air from the Kanawha Valley, WV --- Trip 1 54

TABLES (cont'd.)

Number | Page

16 Estimated Levels of Volatile Organics in Ambient Air from the Kanawha Valley, WV --- Trip 2 55

17 Estimated Levels of Volatile Organics in Ambient Air from the Kanawha Valley, WV --- Trip 3 56

18 Volatile Organics Identified in Ambient Air in the Shenandoah Valley, VA (Front Royal) 58

19 Estimated Levels of Halogenated Organic Vapors in Ambient Air from Front Royal, VA --- Trip 1 63

20 Estimated Levels of Halogenated Organic Vapors in Ambient Air from Front Royal, VA --- Trip 2 64

21 Estimated Level of Halogenated Organic Vapors in Ambient Air from Front Royal, VA --- Trip 3 65

22 Estimated Levels of Volatile Organics in Ambient Air from Front Royal, VA --- Trip 1 66

23 Estimated Levels of Volatile Organics in Ambient Air from Front Royal, VA[a] --- Trip 2 67

24 Estimated Levels of Volatile Organics in Ambient Air from Front Royal, VA[a] --- Trip 3 68

25 Control Samples for each Field Sampling Trip 74

A-1 Overall Theoretical Sensitivity of High Resolution Gas Chromatography/Mass Spectrometry/Computer Analysis for Atmospheric Pollutants 81

A-2 Breakthrough Volumes for Several Atmospheric Pollutants[1]. 89

A-3 Operating Parameters for GLC/MS/COMP System 94

B-1 Estimation of Breakthrough Volumes for Vinyl Chloride and Vinyl Bromide on SKC Carbon (104) 109

B-2 Estimation of Breakthrough Volumes for Methyl Chloride and Methyl Bromide on SKC Carbon (104) 109

B-3 Approximate Limit of Detection for Methyl Chloride, Methyl Bromide, Vinyl Chloride and Vinyl Bromide[a] 111

TABLES (cont'd.)

Number Page

B-4 Parameters for Removing Water and Transferring Vapors to Tenax GC 115

B-5 Operating Parameters for GLC/MS/COMP System 116

C-1 Very Volatile Organic Compounds Identified in Air in the Kanawha Valley, WV (Trip 1, P2/L2) 119

C-2 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 1, P2/L2) 120

C-3 Very Volatile Organic Compounds Identified in the Kanawha Valley, WV (Trip 1, P2/L5) 123

C-4 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 1, P2/L5) 124

C-5 Very Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 1, P2/L6) 126

C-6 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 1, P2/L6) 127

C-7 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 2, P2/L3) 129

C-8 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 2, P2/L4) 132

C-9 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 2, P2/L5) 135

C-10 Very Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 3, P1/L8) 137

C-11 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 3, P1/L8) 138

C-12 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 3, P2/L1) 140

C-13 Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 3, P2/L2) 142

C-14 Very Volatile Organic Compounds Identified in Ambient Air in the Kanawha Valley, WV (Trip 3, P2/L9) 145

TABLES (cont'd.)

Number Page

D-1 Compounds Identified in Polar Neutral Fraction of <1.7μ Air Particulate Collected in Kanawha Valley, WV (Trip 3, L1/L1) 147

D-2 Compounds Identified in PNA Fraction of <1.7 μ Air Particulate Collected in Kanawha Valley, WV (Trip 3, P1/L1) 148

D-3 Compounds Identified in Paraffin Fraction of <1.7μ Air Particulate Collected in Kanawha Valley, WV (Trip 3, P1/L1) . 150

D-4 Compounds Identified in Base Fraction of < 1.7 μ Air Particulate Collected in Kanawha Valley, WV (Trip 3, P1/L1) 151

E-1 Very Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 1, P1/L4). 157

E-2 Very Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 1, P2/L5) 158

E-3 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 1, P3/L2) 159

E-4 Very Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 1, P3/L6) 161

E-5 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 1, P3/L6). 162

E-6 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 2, P2/L3) 164

E-7 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 2, P3/L5) 166

E-8 Very Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 3, P1/L9). 168

E-9 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 3, P2/L8) 169

E-10 Volatile Organic Compounds Identified in Ambient Air in Front Royal, VA (Trip 3, P2/L9) 171

F-1 Compounds Identified in Methanol Extract of <1.7μ Fraction of Air Particulate Collected in Front Royal, VA (Trip 3, P1/L4) . . . 175

F-2 Compounds Identified in Toluene Extract of <1.7μ Fraction of Air Particulate Collected in Front Royal, VA (Trip 3, P1/L4) . . . 177

ACKNOWLEDGEMENTS

The valuable assistance in sample collection, workup, method development, and data interpretation by Ms. S. P. Parks is gratefully acknowledged. Also, field assistance by Mr. C. A. Billings, advice from Dr. C. M. Sparacino, and mass spectral support from Ms. D. Smith, Dr. K. Tomer, Dr. J. T. Bursey, and Ms. N. P. Castillo are greated appreciated.

The sampling of ambient air in the Kanawha Valley was assisted by advice from Mr. Ronald Engle of the West Virginia State Air Pollution Control Commission and the individuals who provided sampling locations.

Sampling in the Shenandoah Valley was assisted by suggestions from Mr. Nick Kappel of the Virginia State Air Pollution Board and the individuals who provided sampling locations.

We wish to thank Messrs. Robert Burton, William Bernard, and Randy Baxter of Environmental Assessment Branch, Health Effects Research Laboratory, EPA, RTP, N. C. for the use of the Massive Air Sampler and the plate scraping facilitites.

Finally, the encouragement and advice from Messrs. Daniel FitzGerald and Ted Erdman of Region III, EPA are deeply appreciated.

SECTION 1

INTRODUCTION

This study is an outgrowth of a long-term research program to develop and perfect a comprehensive and systematic approach to the measurement of organic compounds in ambient air. Previous research has demonstrated that a wide range of atmospheric contaminants may be readily measured by this technique. Until this technique was developed, the ability to collect and analyze a wide variety of chemical classes from the atmosphere containing toxic and/or carcinogenic compounds was not possible. Thus, the health impact of these compounds had not been thoroughly studied. The techniques used in this study enable the characterization of a wide profile of organic compounds in ambient air. These profiles provided a panoramic view of the pollution at specific sites and times.

Organic compounds are present in the atmosphere at widely varying levels and may be either site-specific or ubiquitous. Sources of these compounds include natural emissions, manufacturing, automobile exhaust, dry cleaning, combustion sources and others. To complicate the milieu, atmospheric reactions degrade some compounds and form others.

The data generated by this technique will allow researchers to identify and quantitate a complex mixture of organic air pollutants in order to begin studing the sources, health effects and environmental effects of these compounds.

SECTION 2

SUMMARY AND CONCLUSIONS

This study was designed to measure a wide range of organic pollutants in two industrialized valleys: the Kanawha Valley, WV and the Shenandoah Valley, VA. The Kanawha is heavily industrialized with a wide variety of chemical industry stretching for roughly 40 km. The valley is narrow with high hills providing a well-defined emission reservoir. The metropolitan population is roughly 150,000. Sampling locations were selected at various sites throughout the valley to assess the general levels of organic compounds. In contrast, the Shenandoah is heavily reliant on tourists and its only major chemical industries are a viscose rayon plant and an allied sulfuric acid plant. The valley is broad and ill-defined near Front Royal (population about 10,000) and would not be expected to trap pollution to any great extent. Sampling sites were selected both upwind and downwind of the industrialized area, and in the center of town in order to assess pollution levels in the area.

Very volatile organic compounds in ambient air (e.g., vinyl chloride) were concentrated on carbon cartridges. Volatile organics (e.g., acetone through naphthalene) were collected on Tenax GC sorbent cartridges. Typical sampling volumes for both carbon and Tenax GC samples were 200-600 ℓ of air. Semivolatiles (e.g., polynuclear aromatics) were collected as particulate using a Massive Air Sampler which collected the <1.7 μ respirable particulate fraction of interest on electrostatic precipitation plates. Typical particulate sampling volumes were 20,000-90,000 m^3.

The volatile and very volatile compounds collected on the sorbent cartridges were analyzed by thermal desorption in line with a gas chromatograph/mass spectrometer/computer (GC/MS/COMP). High resolution was achieved using an SE-30 SCOT capillary column. The semivolatile compounds were extracted from the particulate, fractionated and then analyzed by capillary column GC/MS/COMP. Data were interpreted by comparison with known mass spectra from spectral libraries. Selected compounds in the volatile fraction were quantitated using the intensities of selected mass ions.

The volatile compounds identified in the Kanawha Valley (with the number of times observed out of ten samples interpreted) include: vinylidene chloride and/or the dichloroethylene isomer (8), methylene chloride (10), chloroform (10), 1,2-dichloroethane (2), 1,1,1-trichloroethane (8), 1-chlorobutane (1), carbon tetrachloride (8), dichloropropene (1), trichloroethylene (6), 1,2-dibromoethane (2), tetrachloroethylene (9), chlorobenzene (1), dichlorobenzene (8), acetaldehyde (9), benzaldehyde (9), aliphatic aldehydes (11), acetone (10), acetophenone (7), benzophenone (4), 21 other ketones, ethyl acetate (6), seven other esters, isopropanol (2), phenol (7), six other alchols, diethyl ether (5), diphenyl ether (4) and eight other ethers, benzene (9), alkyl benzene, indan (7), indene (1), naphthalene (8), alkyl naphthalenes, biphenyl (7), CS_2 (6), other sulfur-containing compounds, cyanobenzene (1), C_3-alkyl pyridine (1), and many alkanes. Quantitative results included high values of 334 ng/m^3 for methylene chloride, 1536 ng/m^3 for tetrachloroethylene, and 71,778 ng/m^3 for benzene. Compounds identified in the particulate fraction included long-chain alkanes, polycyclic aromatic hydrocarbons (PAH) from naphthalene through anthanthrene (or an isomer), alkyl-PAH derivatives, and nitrogen-containing heterocycles.

In the Shenandoah Valley, VA, the volatile compounds identified (with the number of times observed out of nine samples interpreted) include: vinylidene chloride and/or the dichloroethylene isomer (9), methylene chloride (9), chloroform (9), 1,2-dichloroethane (1), 1,1,1-trichloroethane (3), carbon tetrachloride (6), trichloroethylene (3), tetrachloroethylene (6), dichlorobenzene (5), acetaldehyde (9), benzaldehyde (6), nine aliphatic aldehydes, acetone (9), acetophenone (6), benzophenone (2), three other ketones, ethyl acetate (4), phenol (5), five alkyl phenols, diethyl ether (8), benzene (8), alkyl benzenes, indan (5), naphthalene (6), alkyl naphthalenes, biphenyl (3), and alkanes. Quantitative results include high values of 238,000 ng/m^3 for methylene chloride, 14,500 ng/m^3 for chloroform, 2,933 ng/m^3, 1,1,1-trichloroethane, 2,994 ng/m^3 for tetrachloroethylene, 24,000 ng/m^3 for benzene, and 3,721 ng/m^3 for acetophenone. Semivolatile compounds identified included polycyclic aromatic hydrocarbons (PAH) from naphthalene through $C_{22}H_{12}$, alkyl-PAH derivatives, oxygenated PNAs, (ketone and anhydrides), sulfur heterocyclic PNAs, and aliphatic hydrocarbons.

Many more compounds were identified with greater frequency in the Kanawha Valley than in the Shenandoah Valley. This is especially noticeable in the pollutants potentially arising from industrial activity (halogenated and oxygenated compounds). Many compounds, including the aromatics, result from combustion (*e.g.*, automobile exhaust) or other sources which could be considered ubiquitous. This qualitative comparison is in keeping with the greater industrial diversity and higher population density of the Kanawha Valley.

In contrast to the qualitative data, the quantitative data showed much higher levels of most organic pollutants in the Shenandoah Valley than in the Kanawha Valley. This is espeically noteworthy, since the Shenandoah Valley is broader and well-defined and is therefore not expected be as good an emission reservoir as the Kanawha Valley. The high levels in the Shenandoah Valley were found on both Trips 1 and 2, implying that the levels found are not fortuitous.

SECTION 3
RECOMMENDATIONS

The results of this study indicate the widespread occurrence of organic compounds in ambient air in these two valleys, sometimes at higher levels. Further research may be directed along eight major fronts:

(1) More vigorous sampling protocols could hopefully identify point source polluters for possible regulatory action.

(2) Long-term monitoring of these valleys may provide both mean concentration data and show any trends in levels of compounds. This data could be useful in identifying industrial pollutants and in establishing a data base for future epidemiological studies.

(3) Future studies could integrate this type of air monitoring with sampling and analysis of other media including water, sediment, soil, vegetation, human tissue, mothers milk, etc.

(4) Future studies should more comprehensively study the correlation of meteorology with pollutant levels (i.e., Do concentrations of specific pollutants rise during an inversion?).

(5) Epidemiological studies could begin to attempt to correlate disease incidence (e.g., cancer) with levels of toxic and/or carcinogenic compounds in air and other media to which humans are exposed.

(6) Expansion and perfection of the techniques reported herein could present a more complete picture of the pollution in these valleys.

(7) More research along the lines of this study and the recommendations given above is needed to fully characterize the air pollution associated with industrialized valleys. Future studies should include both industrialized, residential/commercial, and uninhabited valleys. In addition, more samples taken over longer time periods are needed to accurately assess pollutant levels.

(8) Since it appeared that the highest concentrations of some pollutants may have occurred at night, it may be important in future studies to integrate the samples for at least 24 hr and/or take consecutive samples which cover entire 24 hr periods.

SECTION 4

OBJECTIVES

This study was designed to provide information on the general organic air pollutant levels in two industrialized valleys. In specific:

(1) Samples were to be collected at three monthly intervals to assess changes of pollutant levels with time.

(2) Samples were to be collected at locations selected to show general pollutant levels in the valley, especially the levels effecting the human population.

(3) Samples were to be analyzed by gas chromatography/mass spectrometry/computer to provide accurate and positive identification of the compounds present.

(4) Qualitative and quantitative data were to be presented such that EPA, Region III personnel could determine the extent to which organic chemicals may affect the human population in the areas sampled.

SECTION 5
SAMPLING

SAMPLING EQUIPMENT

Due to the wide range of compounds sought, it was necessary to use more than one collection method. Highly volatile compounds were collected on carbon cartridges. Compounds of medium volatility were collected on a polymeric sorbent cartridge (Tenax GC). Particulates were collected on impactor and electrostatic precipitation plates using an ultra-high volume Massive Air Sampler (MAS).

Collection of High- and Medium-Volatility Organics on Carbon and Tenax GC

High and medium volatility materials were concentrated from ambient air on a sampling train consisting of (1) a glass fiber filter (GFF), (2) a cartridge of Tenax GC, and (3) a cartridge of carbon, sequentially.

Glass Fiber Filter (GFF)--

As illustrated in Figure 1, the glass fiber filter (GFF) was placed at the front end of the sampling train, held in place by a 25 mm Delrin filter holder. Gelman Type A-E 25 mm diameter filters were used. These filters are rated at 99.7% efficiency for particles greater than 0.3 μm by the dioctyl phthalate permeation test, and at 98% efficiency for particles of 0.05 μm diameter or larger. The filter was used primarily to exclude particulate containing non-desorbable compounds which would contaminate the Tenax GC.

A series of experiments were conducted to determine whether the GFF excluded chromatographable compounds from the Tenax GC cartridge. Parallel cartridges, with and without the GFF, were sampled near a highway intersection with a large number of diesel trucks starting and stopping (U. S. 70 and Old U. S. 70, Bethesda, NC). Gas chromatographic analysis with flame ionization detection (GC/FID) of these two cartridges yielded similar gas

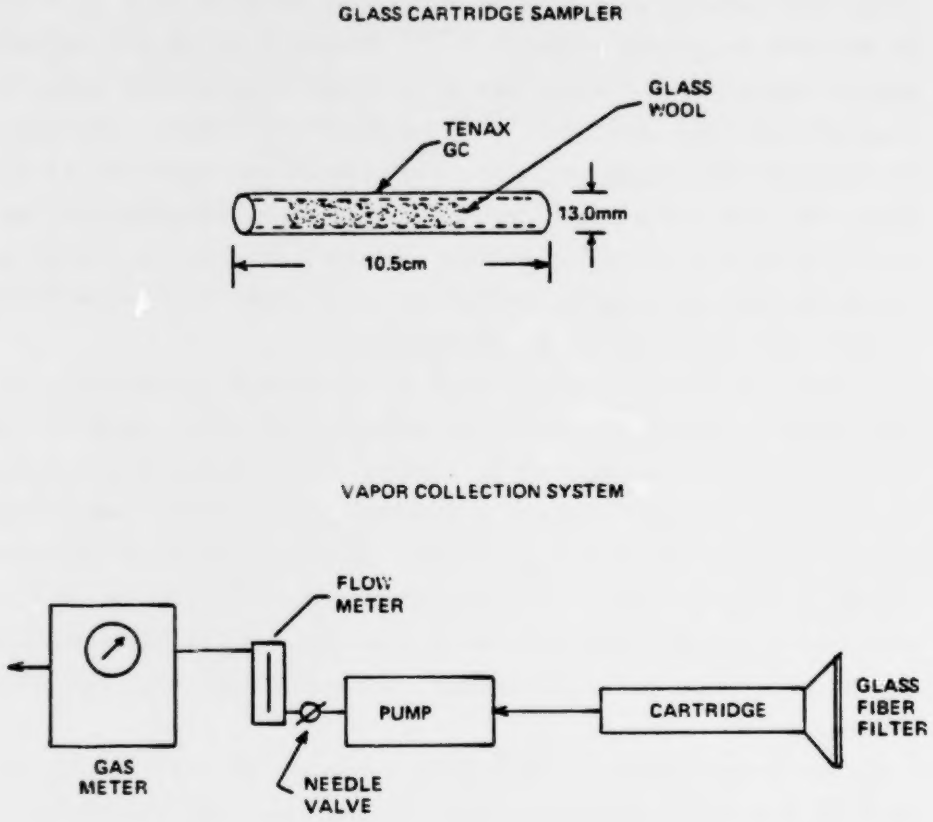

GLASS CARTRIDGE SAMPLER
GLASS WOOL
TENAX GC
13.0mm
10.5cm
VAPOR COLLECTION SYSTEM
FLOW METER
PUMP
CARTRIDGE
GLASS FIBER FILTER
GAS METER
NEEDLE VALVE

Figure 1. Collection system for concentrating high and medium volatility organic compounds from ambient air.

chromatograms, indicating no desorbable compounds were being excluded from the Tenax GC cartridge by the GFF. Based on these results, the GFF was retained in the sampling train, since its use allowed recycling of the Tenax GC resin.

Tenax GC Sampling Cartridges--

The sampling tubes were prepared by packing a 10 cm x 1.5 cm i.d. glass tube containing 6.0 cm of 35/60 mesh Tenax GC (1.6 g) with glass wool in the ends to provide support.(1-3) Virgin Tenax GC was extracted in a Soxhlet extractor for a minimum of 18 hours with acetone prior to preparation of cartridge samplers.(1,2) In those cases where sampling cartridges of Tenax GC were being recycled, the sorbent was extracted in a Soxhlet apparatus with acetone, as described for the virgin material, and also extracted with a non-polar solvent, hexane, in order to remove the relatively non-polar and non-volatile materials which might have accumulated on the sorbent bed during previous sampling periods.

After purification, the Tenax GC was meshed to provide a 35/60 particle size range. Cartridges were then prepared and conditioned at 270°C with helium flow at 30 ml/min for 20 minutes. The conditioned cartridges were transferred to Kimax® (2.5 cm x 150 cm) culture tubes, immediately sealed using Teflon-lined caps, and cooled. This procedure was performed in order to avoid recontamination of the sorbent bed.(1,2) One or more cartridges selected at random from each batch were checked for background using GC/FID. If the background was unacceptable, the cartridges were redesorbed and checked again.

For large sample volumes it is important to realize that elution of certain organic compounds through the sampling tube will occur if their breakthrough volume is exceeded. The breakthrough volume is defined as that point at which 50% of a discrete sample introduced into the cartridge is lost. The breakthrough volumes of some representative compounds are shown in Appendix A.(1,2,4,5,6) These breakthrough volumes have been determined by a previously described technique.(1,4) Although the identity of a compound during ambient air sampling is not known (therefore, also its breakthrough volume) the compound can still be quantitated after identification by GC/MS/COMP once the breakthrough volume has been established.

Thus, the last portion of the sampling period represents the volume of air sampled prior to breakthrough. For cases when the identity of the compound is not known until after GC/MS/COMP analysis, the breakthrough volume is determined after the fact and the quantitation accomplished as above.

Previous experiments have shown that organic vapors collected on Tenax GC sorbent are stable and can be quantitatively recovered from the cartridge samplers up to four weeks after sampling when they are tightly closed in cartridge holders, protected from light, and stored at 0°C.(1)

Carbon Cartridges--

High purity charcoal (SKC, Inc., Pittsburgh, PA) was packed into a bed, 3 x 0.3 cm, in a glass tube. Carbon from this source has been shown to be pure for these applications and was used without solvent purification. Carbon cartridges were thermally stripped of organic vapors by heating to 400°C under He flow for 30 min.

These cartridges efficiently trap the organic compounds which pass through the Tenax GC cartridge (vinyl chloride, vinyl bromide, methyl chloride, and methyl bromide). They have been successfully used to analyze vinyl chloride and the other highly volatile halocarbons (b.p. <30°) which are not retained on Tenax GC to any significant extent.(7) The breakthrough volume for vinyl chloride, and thus the amount collectable, on the carbon cartridges is about 20 times that of Tenax GC.

Sampling Apparatus--

Continuous sampling of ambient air was accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Figure 1). The flow was monitored through a calibrated rotameter, and the total flow registered by a dry gas meter. Concomitant with these parameters, the temperature was also noted, since it was important for establishing the breakthrough volume and therefore the total sampling volume which can be used for quantitation. This portable sampling unit operated on a 12-volt storage battery and was operated from 4-12 hrs, depending on the sampling conditions and flow rates used. Duplicate cartridges were deployed on each sampling unit. A total of four portable sampling units were available for sampling.

At the same location as the MAS (vide infra), a duPont Model P-200 personnel sampler was used to continuously sample air onto carbon and Tenax GC cartridges over the entire period that the MAS was operated. The duPont personnel sampler, operated at about 200 cc/min, was powered by a 6V lantern battery and the entire sampler housed in a chrome-plated aluminum box.

Collection of Low-Volatility Organics Using a Massive Air Sampler (MAS)

A Massive Air Sampler (MAS) manufactured by Battelle Memorial Institute, Columbus, OH(8,9) was used for collecting particulate fractions in the 3.5 - 20, 1.7 - 3.5 and <1.7 micron ranges. Preliminary studies (personal communication R. Burton, Environmental Assessment Branch, HERL, USEPA, RTP, NC) indicated that the larger particle range yielded greater than 1 g in a 100 hr collection period at an 18 m^3/min sampling rate. The middle sized particle range was found to be approximately 0.8 g while the smallest particles were well over 3 g for this collection period and rate.

The sampler, about 140 cm tall and 60 cm square, is a large cascade impactor with electrostatic precipitation for collection of the fine particulate which is not impacted. Air is sampled at a rate of 630 cfm (18 m^3/min) by a blower using a 750j/sec motor (115 V, 12 amps). The air enters the sampler over a lip enclosed by the cover which serves as a scalping stage with a cutoff of about 20 μ. The air then enters the impactor assembly stages consisting of four Teflon-coated plates (28 x 43 cm). The first and third plates have slots which serve as impactor jets. The second and fourth plates are the collection target plates located about 1 cm below the jet plates. Below the impactor sections is the electrostatic precipitator, consisting of ionizing wires (-10 kV) and 55 Teflon-coated collection plates (28 x 43 cm). The plate potential is adjusted to the maximum achievable without excessive arcing (generally 5-7 kV, depending on the humidity). From the electrostatic precipitation section, the air is drawn to the blower and then to exhaust. The control panel consists of a magnahelic vacuum gauge to register the flow, a run time meter (in hours), a volt meter to indicate the voltage applied across the precipitator plates, and a red flashing light to indicate malfunctions.

For the purpose of this study, the MAS was chained into a pickup truck for transportation and left in situ during sampling.

Upon return from the field, the impactor and electrostatic precipitator plates were scraped into glass vials, kept in the dark, and stored under nitrogen at -5° to retard chemical reactions. The plates were scraped in a specially designed glove box to prevent contamination of the sample and for protection of personnel.

METEOROLOGY

Continuous measurements of temperature, wind direction and wind run were recorded on a MRI (Meteorological Research, Inc. Altadena, California) Mechanical Weather Station (MRI) at a central location through the sampling period. The strip chart record allowed subsequent reference to calm periods, wind direction shifts, etc., which could affect sampling results. Intermittent measurements were made at each sampling location. Humidity, temperature, wind speed, and wind direction were measured and noted along with general conditions (rain, snow, cloud cover, odors, etc.). Measurements at each location provided a cross-check with the MRI record.

Pertinent meteorological data for the sampling period were obtained from the nearest National Weather Service office. This data was used to augment that obtained at the sampling location.

SAMPLING PROTOCOLS

Samplers were set out at locations designated in a numercial sequence (e.g. L1) for a sampling period (e.g. P1). Thus, each sample is designated by a unique Trip/Period/Location (e.g. Trip 1, P2/L6) code. This code is presented in the sampling protocol tables and then used to identify samples in the analytical results.

SAMPLING LOCATIONS

Kanawha Valley

Many manufacturers of organic chemicals which, along with the by-products, are potentially toxic, carcinogenic and/or teratogenic are located in the Kanawha Valley, W.V. (Figure 2). DuPont, near Belle, has a large chemical complex for the synthesis of substances such as methyl-methacrylate, methylamines, ammonia, hydrogen cyanide, herbicides, and insecticides. In South Charleston are production and consumption plants (Union Carbide,

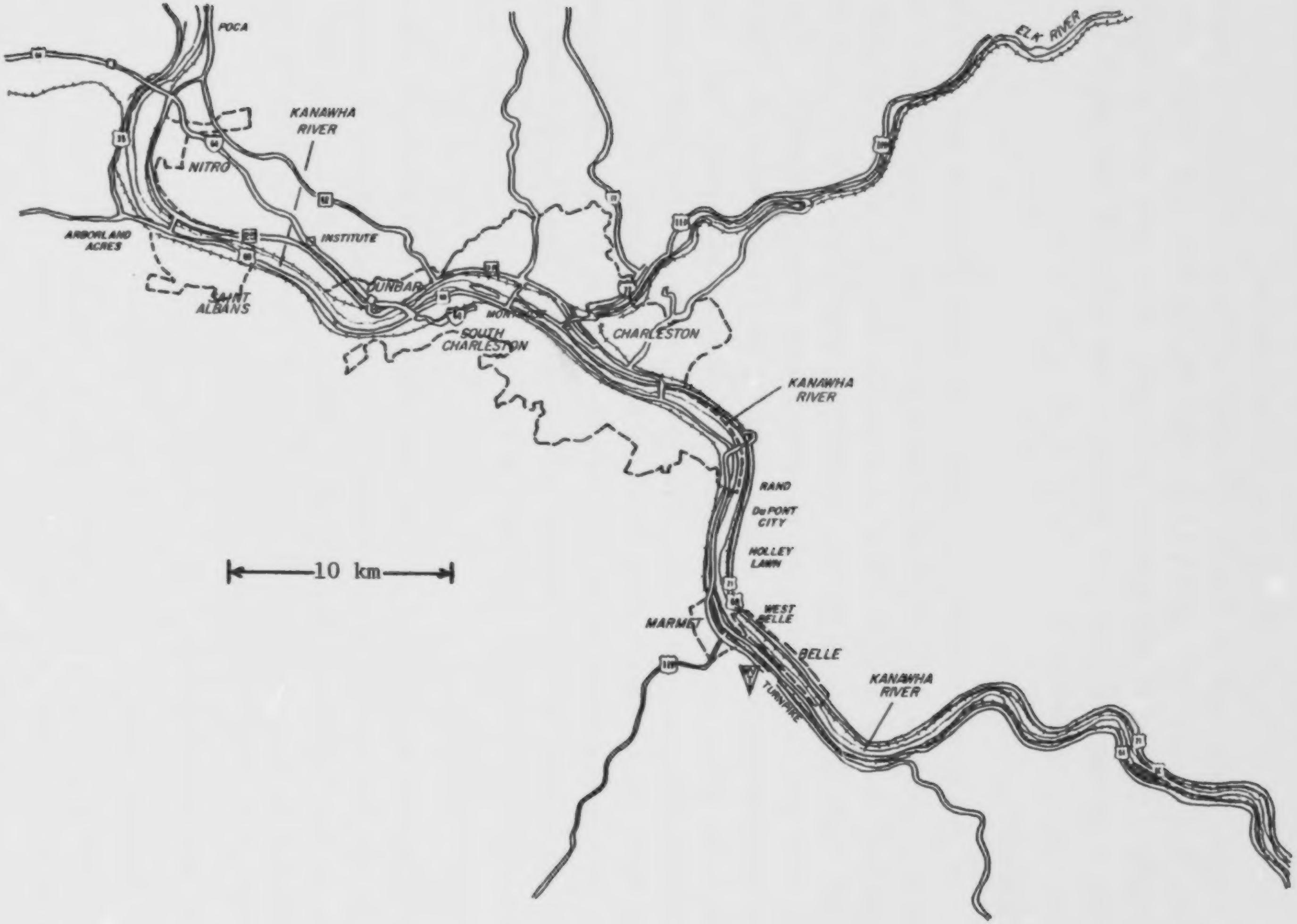

POCA
KANAWHA RIVER
NITRO
INSTITUTE
ARBORLAND ACRES
SAINT ALBANS
DUNBAR
SOUTH CHARLESTON
CHARLESTON
ELK RIVER
KANAWHA RIVER
RAND
DuPONT CITY
HOLLEY LAWN
WEST BELLE
MARMET
BELLE
TURNPIKE
KANAWHA RIVER
10 km

Figure 2. The Kanawha River Valley, West Virginia.

and FMC). Plastics, PVC, antifreeze, chlorine, halogenated organics, carbon disulfide, peroxides, etc. are the predominant chemicals produced here. The major facility in the town of Institute is Union Carbide which also processes a broad spectrum of compounds, e. g., viscose rayon, and phthalate esters. There is also a large scale olefin processing complex and a rubber accelerator plant. A major terminal loading facility in South Charleston handles large quantities of a variety of organic compounds. Monsanto, FMC, Allied, and Fike have plants near Nitro for the production of antioxidants, rubber accelerators, industrial chemicals, and other materials. Several other chemical manufacturers, consumers, and transporters are located in the Kanawha Valley, some or all of which may contribute to the presence of organic materials in the ambient air.

Previous sampling and analysis efforts have found a wide variety of organic compounds in ambient air.(1,10,11) These results were used in part to select locations for sampling during this study.

The rationale for selection of the locations in the Kanawha Valley was to place samplers at several points along the valley floor throughout the industrialized, metropolitan Charleston, WV area. The location was selected within a general area by sampling personnel on the basis of estimates on where high concentrations of air pollutants might be detected, the potential for human exposure, security of personnel and equipment, and also approval of property owners where applicable.

The MAS, duPont sampler, and MRI weather station were located at the North Charleston Community Center (21st St. W. and 7th Ave., W.) based on recommendations from personnel in the Environmental Assessment Branch, HERL, EPA, RTP, NC who had sampled there previously with the MAS. This location provided not only power, but fenced-in areas for security. Centrally located in the valley, this location was judged to provide "average" meteorology and air samples.

The other four samplers were located up and down the valley at locations in Belle, South Charleston, St. Albans or Institute, and Nitro.

The sampling locations, times, volumes, and meteorology are summarized in Tables 1-4. The location numbers are shown on detailed maps (Figures 3-6).

Table 1. SAMPLING LOCATIONS IN THE KANAWHA VALLEY, WV.

Location	Site	Address	Remarks
L1	Charleston	4th Ave. W. and 21st St. W.	North Charleston Recreation Center. [MAS located at Maintenance Steel near west entrance; MRI and duPont samples located around swimming pool.
L2	S. Charleston	314 4th Ave.	S. Charleston Fire Department Sample located on upper level roof.
L3	St. Albans	6500 MacCorkle Ave. S.W.	Riverside Nursing Home. Sampler located on river bank in open area.
L4	Nitro	N.W. of intersection of W.V. 25 and I-64.	Nitro Sewage Treatment Plant. Sampler located along fence, upwind of all sewage treatment facilities.
L5	W. Belle		Marmet Dam and Locks. Sampler located on hill above parking lot.
L6	Nitro	2009 20th St.	Nitro Fire Department. Sampler located on roof.
L7	Nitro	4107 1st Ave.	Front yard of private residence, directly across street from chemical manufacturing facilities.
L8	Institute	Barron Dr. between 4th St. and Curtis Sq.	Back yard of private residence.
L9	Nitro	N.W. of intersection of W.V. 25 and I-64.	South side of United Distribution Service parking lot.

Table 2. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN KANAWHA VALLEY, WV --- TRIP 1

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks[*]
Charleston	P1/L1	1030-1435 (9/27 - 9/28)	29,500,000[a]	T[b]= 7°C to 20°C. Winds: S.S.W. to W./calm to 2.8 m/s.
Charleston	P1/L1	1020-1435 (9/27 - 9/28)	258[c]	At 0955 (9-27), RH[d] = 85%, T = 19°C, low cloud cover.
S. Charleston	P1/L2	1115-1617	597	T = 22°C, RH = 72%, low cloud cover.
St. Albans	P1/L3	1202-1715	537	T = 17°C to 20°C. Winds: S.S.W. to W.S.W./1.4 to 28 m/s. Rain for 1 hour.
Nitro	P1/L4	1400-1610	497	T = 18°C to 20°C. Winds: S.W./1.7 to 2.8 m/s.
W. Belle	P1/L5	1349-1945	564	T = 18°C to 20°C. Winds: S.W./1.7 to 2.8 m/s.
S. Charleston	P2/L2	0825-1308	558	T = 8°C to 13°C. Winds: W. to S.W./0.5 to 1.7 m/s.
St. Albans	P2/L3	0715-1355	710	T = 8°C to 15°C. Winds: W. to S.W./calm to 1.7 m/s.
W. Belle	P2/L5	0740-1555	541	T = 7°C to 20°C. Winds: W. to S.W./0.5 to 1.7 m/s.
Nitro	P2/L6	0930-1320	410	T = 9°C to 13°C. Winds: W. to S.W./1.1 to 1.7 m/s; overcast.

[a] Sample collected with MAS
[b] Temperature
[c] Long-term samples taken with small duPont personal sampling pump.
[d] Relative humidity

[*] General weather conditions for 9/27 and 9/28: Cool, skies overcast with periods of intermittent light rain and slow but steady showers. Winds: calm to light breezes.
Date: 9/27-28/77

Table 3. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN KANAWHA VALLEY, WV --- TRIP 2

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks*
Charleston	P1/L1	0910-0820 (10/24-10/26)	49,700,000[a]	T[b] = 7°C to 23°C, RH[c] = 31% to 91%. Wind: E.S.E./calm to 7 m/s.
Charleston	P1/L1	0925-0850 (10/24-10/26)	512[d]	At 0910 (10-24), T = 10.5°C, RH = 87%, partly cloudy. Eight hours of light rain during sampling time T = 13°C to 22°C[f], RH = 35% to 93%[f]. Winds: E.S.E. to E.[f]/calm to 6 m/s[f].
S. Charleston	P1/L2	1200-1737	268	T = 23°C to 18°C. Winds: S. to E.S.E./1.1 to 5 m/s. At 1151, T = 23°C, RH = 32%, slightly hazy, no odors.
St. Albans	P1/L3	1130-1635	370	T = 17°C to 23°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1125, T = 17°C, RH = 54%, low haze, no odors.
Nitro	P1/L4	1035-1600	322	T = 17°C to 23°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1030, T = 17°C, RH = 68%; hazy, strong odor.
W. Belle	P1/L5	1315-1808	414	T = 23°C to 17°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1313, T = 23°C, RH = 50%; hazy, slight odor.
S. Charleston	P2/L2	0632-1205	297	T = 14°C to 18°C. Winds: E. to S.E./calm to 4 m/s. RH = 58% to 69%.
St. Albans	P2/L3	0534-1147	432	T = 14°C to 18°C. Winds: E. to S.E./calm to 4 m/s. At 0533, T = 14°C, RH = 88%; overcast, strong odor. RH = 55% to 72%[f].
Nitro	P2/L4	0505-1118	410	T = 14°C to 17°C. RH = 55% to 72%[f]. Winds: E. to S.E./calm to 4 m/s. Overcast, strong odor. At 0505, T = 18°C[e], RH = 79%.
W. Belle	P2/L5	0600-1235	569	T = 13°C to 18°C. RH = 55% to 72%[f]. Winds: E. to S.E./calm to 4 m/s. At 0555, T = 13°C. Overcast, no odor. RH = 69% to 54%.

---

[a] Sample collected with MAS.

[b] Temperature.

[c] Relative humidity.

[d] Long-term sample collected with duPont personal sampling pump.

[e] Temperature beside sewage treatment plant settling ponds -- somewhat higher than ambient.

[f] Data from National Weather Service Forecast Office, Kanawha Airport, Charleston, WV.

[*] General weather conditions for 10/24 through 10/26: Cool, skies clear with low-lying haze changing to overcast with some light shower activity. Winds generally calm to moderate from the S.E. to S.W.

Dates: 10/24-26/77

Table 4. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN KANAWHA VALLEY, WV --- TRIP 3

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks*
Charleston	P1/L1	1910-0917 (11/16-11/20)	90,800,000^{a}	Odors: occasionally strong chemical. At 1005 (11-17) RH^{e}= 63%. At 1125 (11-18) RH = 38%. T^{c} = 2 to 15°C^{f}, RH = 28% to 100%^{f}. Winds: S.W. to N. to E.^{f}/calm to 11 m/s.^{f}
Charleston	P1/L1	1910-1125 (11/16-11/18)	344^{b}	T = 4°C to 15°C^{f},RH = 31%-80%^{f}. Winds: S. to W./2-11 m/s^{f}.
S. Charleston	P2/L2	1235-1737	1087	T = 11°C to 9°C. Wind: W.S.W./6 to 10 m/s. RH= 31% to 44%^{f}.
W. Belle	P2/L5	1348-1811	1205	T = 11°C to 9°C. Wind: W.S.W./4 to 10 m/s. RH= 31% to 44%^{f}.
Nitro	P2/L7	1335-1725	480^{d}	T = 11°C to 10°C. Wind: W.S.W./4 to 10 m/s^{f}. At 1335 and 1720, odor strong. RH = 31% to 44%^{f}.
Institute	P2/L8	1235-1700	861	T = 11°C to 10°C. Wind: S.W.S./6 to 10 m/s. At 1235 and 1700, odor acrid, of rotting walnuts. RH=31% to 44%^{f}.
Charleston	P3/L1	1135-0930 (11/18-11/20)	331^{b}	At 1125 (11-18), T = 10°C, RH^{e} = 38%, sky clear. T= 1°C to 15°C^{f}, RH=28% to 100%^{f}. Wind: S.W. to N.to E.^{f}/calm to 6 m/s^{f}.
S. Charleston	P3/L2	0809-1310	1096	T = 4 to 9°C^{f}, RH=49% to 33%^{f}. Wind: W.S.W.^{f}/4 to 8 m/s^{f}.
W. Belle	P3/L5	0729-1241	1084	T = 4 to 9°C^{f}, RH=49% to 33%^{f}. Wind: W.S.W.^{f}/4 to 8 m/s^{f}.
Institute	P3/L8	0728-1210	743	Odor of rotting walnuts, naphthalene or mothballs. T = 4 to 9°C^{f}, RH=49% to 33%^{f}. Wind: W.S.W.^{f}/4 to 8 m/s^{f}.
Nitro	P3/L9	0802-1250	953	Strong odor. T = 4 to 9°C^{f}, RH=49% to 33%^{f}. Wind: W.S.W.^{f}/4 to 8 m/s^{f}.

[a] Sample collected with MAS

[b] Long-term sample collected with duPont personal sampling pump.

[c] Temperature

[d] Pump malfunctioned during sampling period.

[e] Relative humidity.

[f] Data from National Weather Service Forecast Office, Kanawha Airport, Charleston, WV.

* General weather conditions for 11/16 through 11/20: Temperatures cool. Skies clear to partly cloudy with very small amount of rain. Winds very brisk with occasional gusts, diminishing to calm on 11/20.

Dates: 11/16-20/77

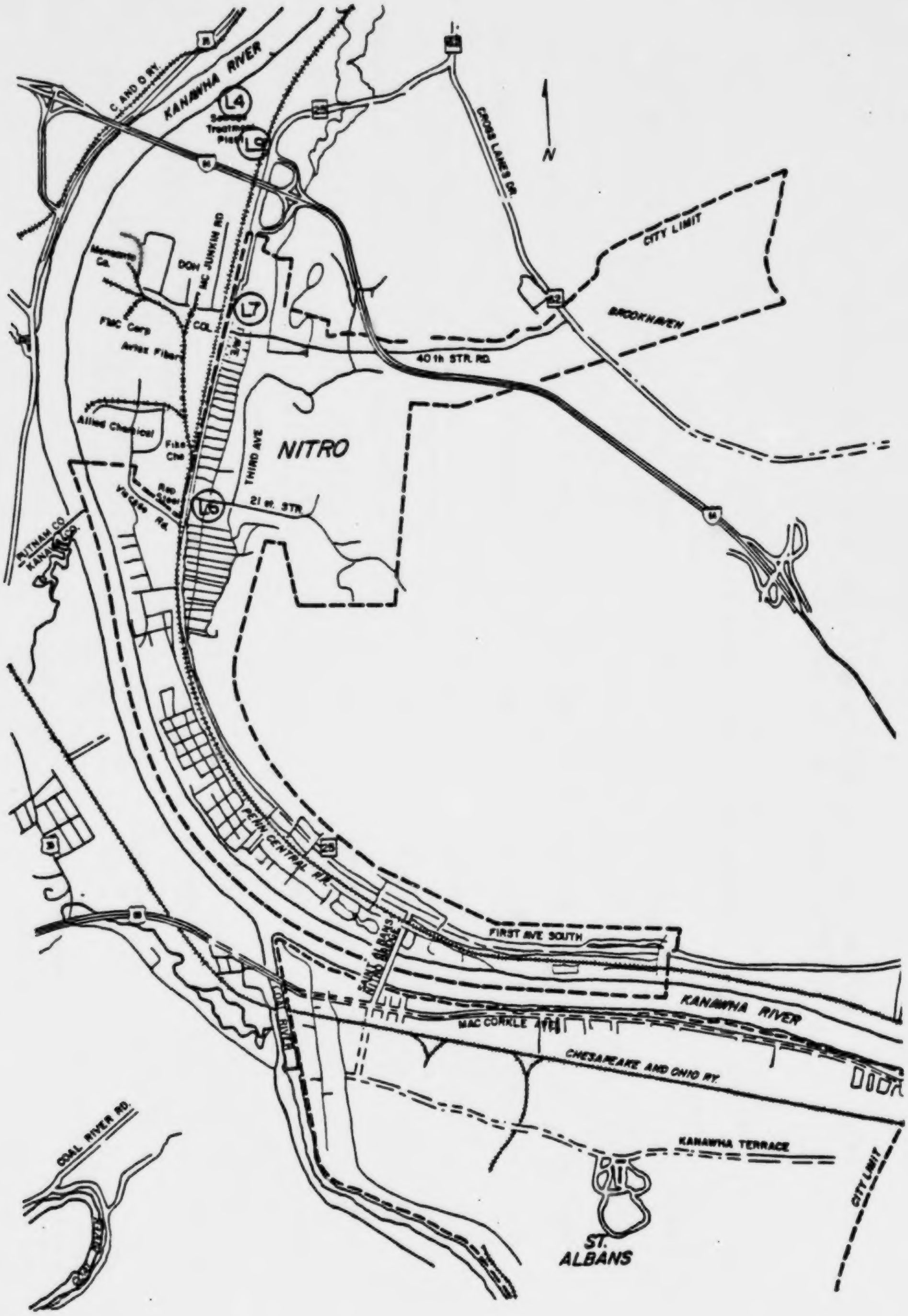

C AND O RY.
KANAWHA RIVER
L4
Sewage Treatment Plant
L9
CROSS LANES DR.
N
CITY LIMIT
BROOKHAVEN
MC JUNKIN RD
Monsanto Co.
DOW
L7
FMC Corp
COL.
Avtex Fiber
40th STR. RD
Allied Chemical
Fiber Che
NITRO
THIRD AVE
Red Steel
Vulcan Rd.
L6
21 st. STR
PUTNAM CO
KANAWHA CO.
PENN CENTRAL R.R.
FIRST AVE SOUTH
KANAWHA RIVER
MAC CORKLE AVE
CHESAPEAKE AND OHIO RY.
KANAWHA TERRACE
CITY LIMIT
ST. ALBANS
COAL RIVER RD.
COAL RIVER

Figure 3. Map of area around Nitro, WV showing L4, L6, L7, and L9 (See Table 1).

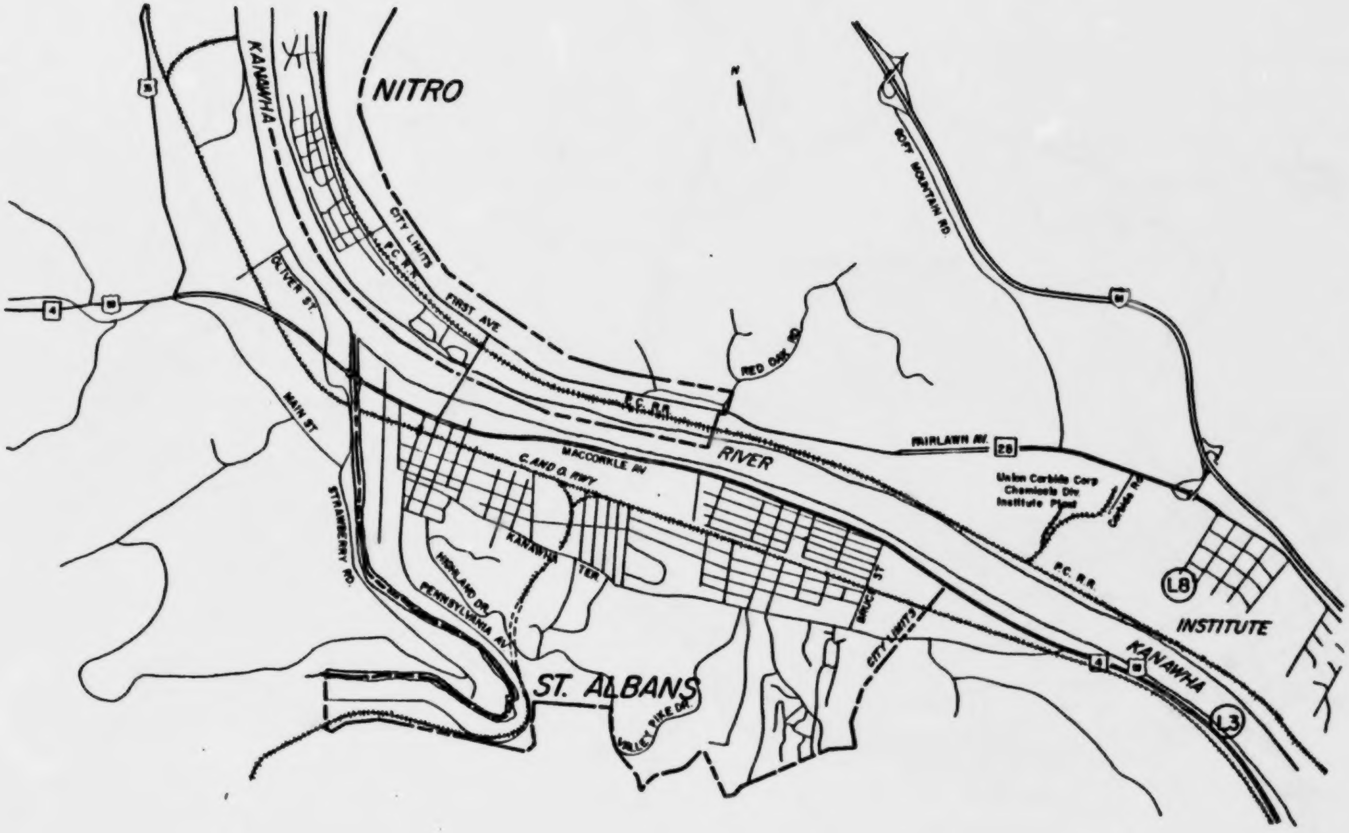

NITRO
KANAWHA
CITY LIMITS
P.C. R.R.
FIRST AVE
OLIVER ST.
MAIN ST
STRAWBERRY RD.
HIGHLAND DR.
PENNSYLVANIA AV
KANAWHA TER
C AND O RWY
MACCORKLE AV
RIVER
P.C. RR.
RED OAK RD
SOFT MOUNTAIN RD.
FAIRLAWN AV.
25
Union Carbide Corp
Chemicals Div
Institute Plant
Carbide Rd
P.C. R.R.
L8
INSTITUTE
KANAWHA
L3
ST. ALBANS
VALLEY PIKE DR
CITY LIMITS
BRUCE ST
N
4

Figure 4. Map of area around St. Albans and Institute, WV showing L3 and L8 (See Table 1).

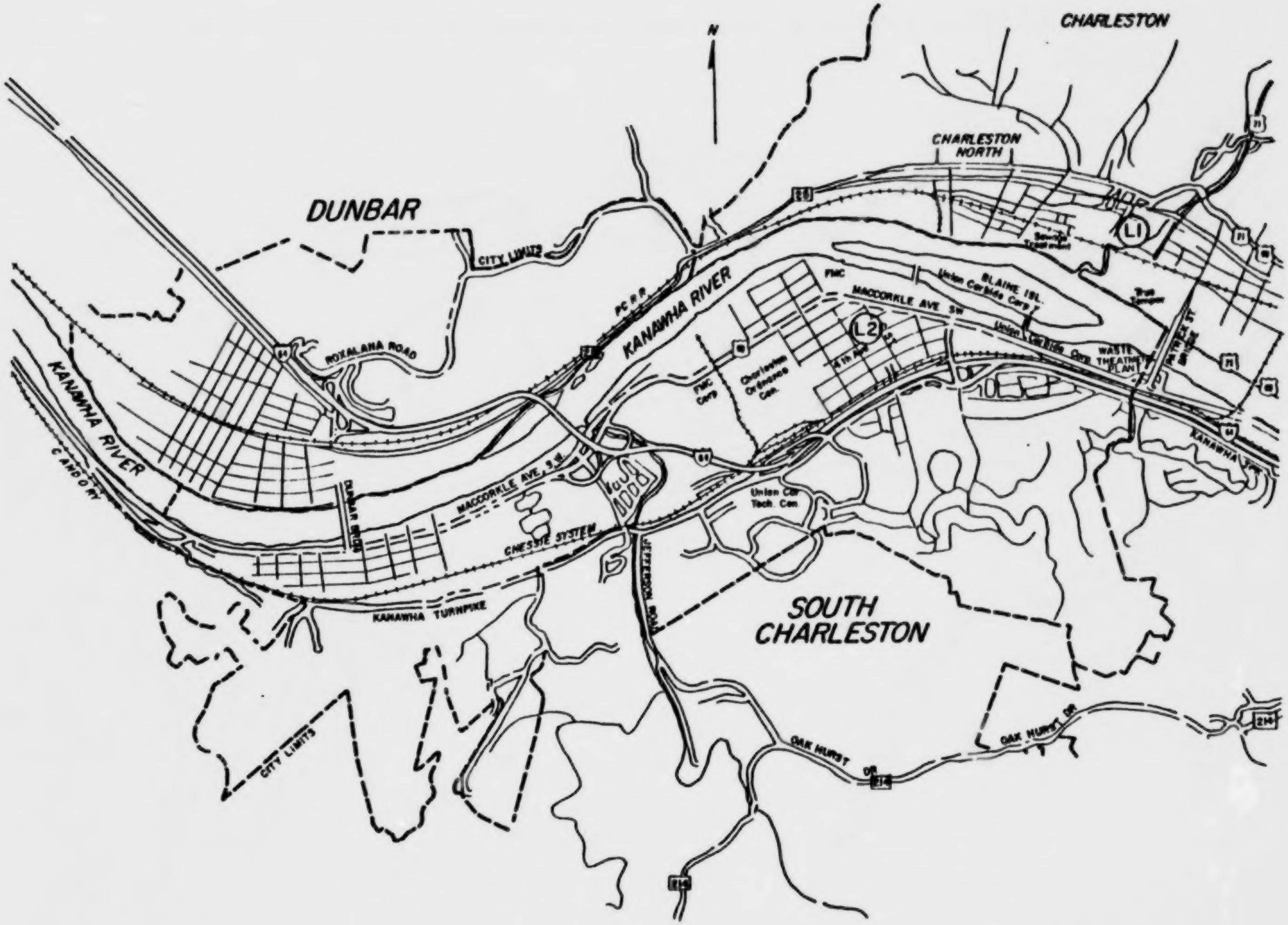

CHARLESTON
N
CHARLESTON NORTH
DUNBAR
CITY LIMITS
L1
L2
KANAWHA RIVER
P C R R
ROYALANA ROAD
BLAINE ISL.
Union Carbide Corp
FMC
MACCORKLE AVE SW
Union Carbide Corp
WASTE TREATMENT PLANT
FMC Corp
Charleston Ordnance Cen.
4th Ave
MACCORKLE AVE S.E.
CHESSIE SYSTEM
Union Car Tech. Cen
JEFFERSON ROAD
KANAWHA TURNPIKE
KANAWHA TPK
DUNBAR BRIDGE
KANAWHA RIVER
C AND O RY
SOUTH CHARLESTON
OAK HURST DR
CITY LIMITS
214
64
60
21
119

Figure 5. Map of area around Charleston and South Charleston, WV showing L1 and L2 (See Table 1).

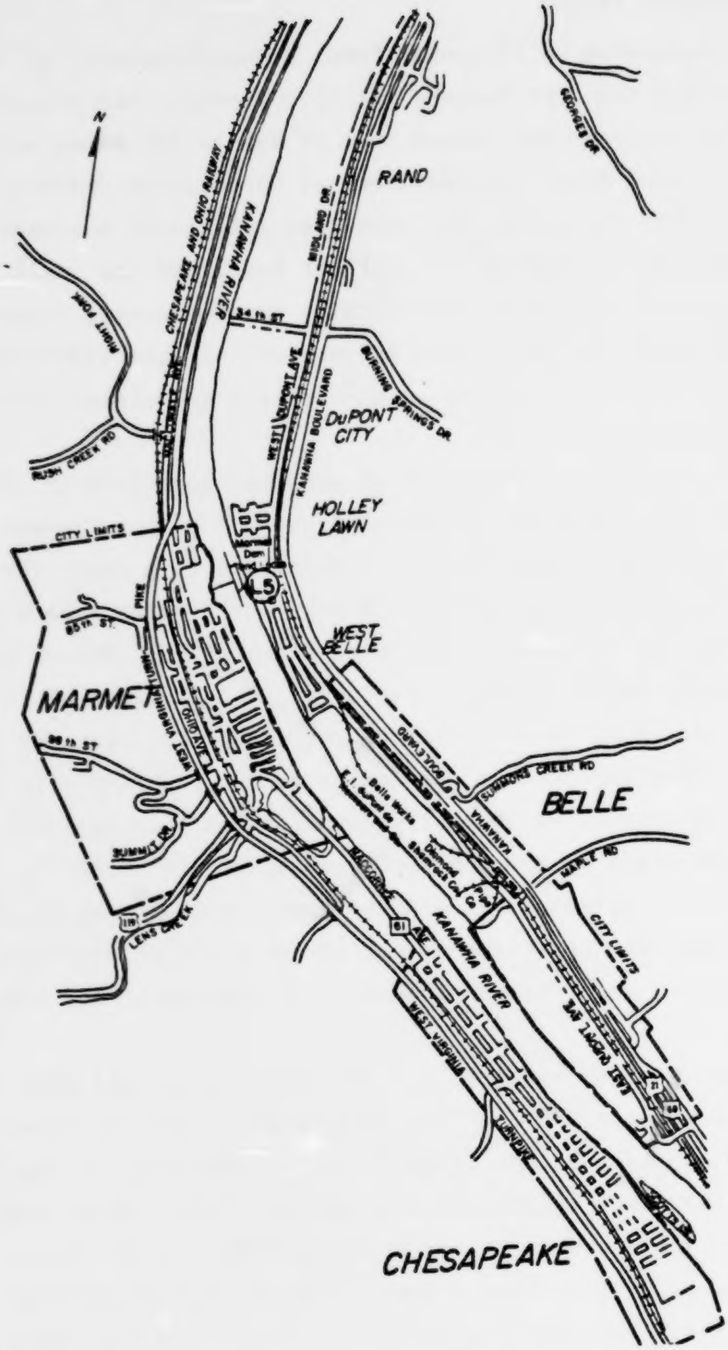

N
GEORGES DR
RAND
CHESAPEAKE AND OHIO RAILWAY
KANAWHA RIVER
MIDLAND DR
34th ST
RIGHT FORK
BURNING SPRINGS DR
WEST DUPONT AVE
KANAWHA BOULEVARD
DuPONT CITY
RUSH CREEK RD
HOLLEY LAWN
CITY LIMITS
L5
WEST BELLE
85th ST
PIKE
MARMET
WEST VIRGINIA TURNPIKE
OHIO AVE
86th ST
KANAWHA BOULEVARD
SIMMONS CREEK RD
BELLE
Belle Works
E. I. duPont de Nemours and Co.
Diamond Shamrock Co.
SUMMIT DR
MAPLE RD
119
LENS CREEK
61
AVE
KANAWHA RIVER
CITY LIMITS
EAST DUPONT AVE
WEST VIRGINIA TURNPIKE
CHESAPEAKE

Figure 6. Map of area around W. Belle, WV showing L5 (See Table 1).

Shenandoah Valley

The Shenandoah Valley, near Front Royal, Virginia, is less highly industrialized than the Kanawha Valley. However, the potential for man-made pollution above and beyond that of day-to-day human activity does exist. In Front Royal, Allied Chemical Corporation operates an organic chemicals plant and Avtex, Inc. produces cellulosic man-made fibers. The other manufacturers listed(12) in Front Royal and the small towns in the vicinity include fabric mills, clothing manufacturers, canneries, producers of crushed rock, and printers. Because of its size (2200 employees), the Avtex plant may be assumed to be the primary industrial source of organic compounds in ambient air.

The rationale for selection of sampling locations in the Shenandoah Valley, VA was completely different from that in the Kanawha Valley, WV. The only large industrial area of interest to this study (by direction of the project officer) was in Front Royal, where Avtex fibers and Allied Chemical Co. are located on adjoining plant sites. Since the sampling area was relatively small (Figure 7) and organic pollutants of interest were suspected of coming from a point source, sampling locations were chosen in a general array surrounding this point source. During each sampling period, locations were selected generally downwind (as determined by smell and the direction of stack emission plumes) and upwind for control. As with the Kanawha Valley, personnel determined sampling locations based on estimates of where high concentrations of pollutants might be detected, potential for human exposure, security of personnel and equipment, and other factors as necessary.

The MAS, duPont sampler, and MRI weather stations were located in downtown Front Royal at the fire department. With personnel on duty full time, this represented the safest location available in the area which also fulfilled the power requirements of the MAS. The duPont sampler and the MRI weather station were placed atop the fire station (about 10 m elevation).

The sampling locations, times, volumes, and meteorology are summarized in Tables 5-8. The location numbers in Tables 5-8 are shown on a detailed map (Figure 8).

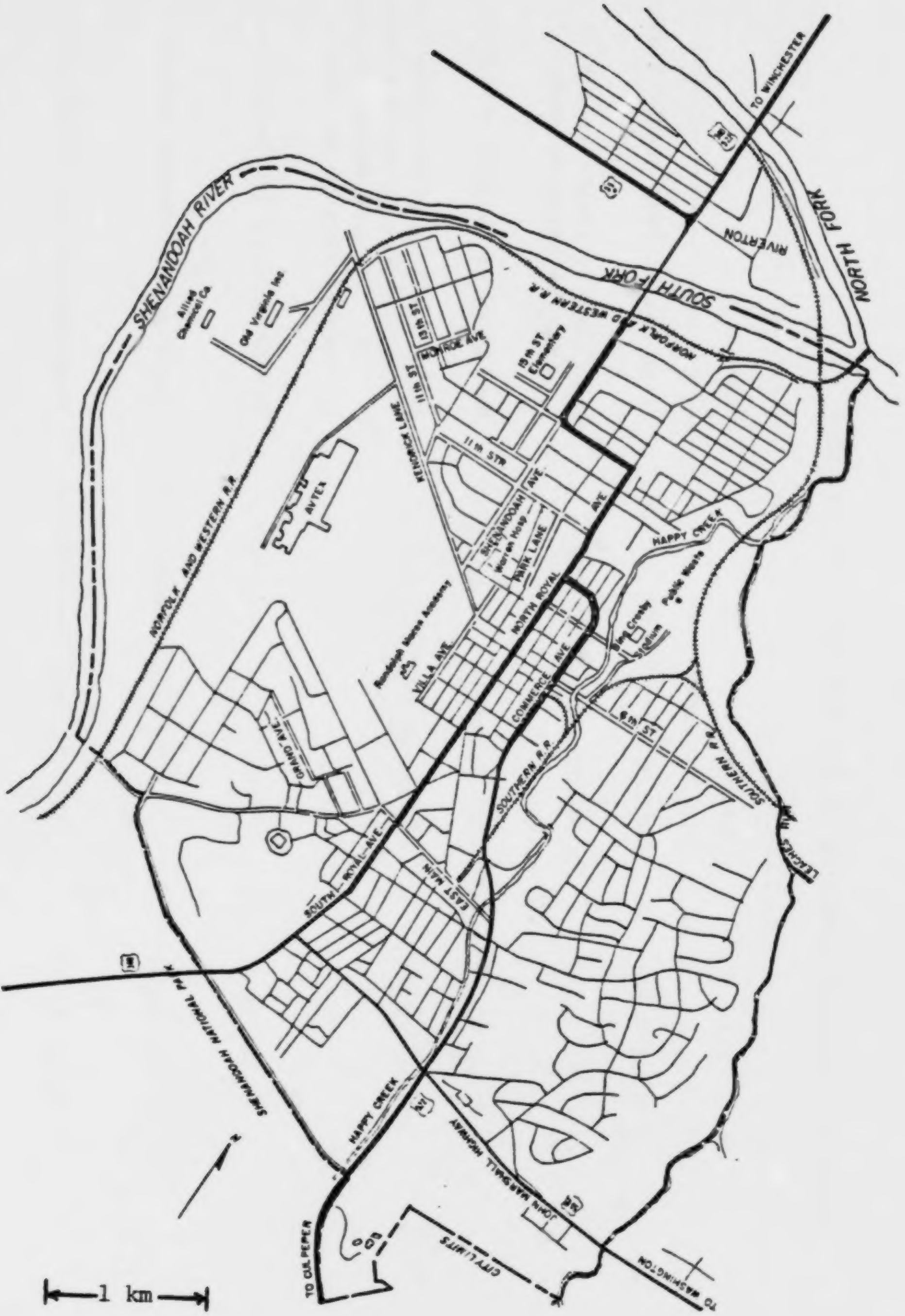

SHENANDOAH RIVER
SOUTH FORK
NORTH FORK
RIVERTON
TO WINCHESTER
NORFOLK AND WESTERN R.R.
Allied Chemical Co
Old Virginia Ind
AVTEX
13th ST
MONROE AVE
11th ST
15th ST Elementary
11th STR
KENDRICK LANE
SHENANDOAH AVE
PARK LANE
NORTH ROYAL AVE
VILLA AVE
COMMERCE AVE
HAPPY CREEK
Public Works
SOUTHERN R.R.
8th ST
LEACH RUN
SOUTH ROYAL AVE
EAST MAIN
SHENANDOAH NATIONAL PARK
JOHN MARSHALL HIGHWAY
CITY LIMITS
TO CULPEPER
TO WASHINGTON
N
1 km

Figure 7. Front Royal, VA.

Table 5. SAMPLING LOCATIONS IN THE SHENANDOAH VALLEY, VA.

Location	Site	Address	Remarks
L1	Front Royal	8th St. and Crosby Rd.	Press box at Bing Crosby Stadium.
L2	Front Royal	3rd St. and Villa Ave.	West side of tennis courts at Randolph Macon Academy.
L3	Front Royal	501 Grand Ave.	Back yard of private residence.
L4	Front Royal	Commerce Ave. between 4th St. and 5th St.	Front Royal Volunteer Fire Dept. MAS located on north parking lot. MRI and duPont personal sampler located on roof.
L5	Front Royal	Commerce Ave. and John Marshall Hwy.	Behind Quality Inn Motel.
L6	Front Royal	13th St. and Commonwealth Ave.	South side of tennis courts.
L7	Front Royal	13th St. and Commonwealth Ave.	Commonwealth Ave. playground.
L8	Front Royal	346 10th St.	Back yard of private residence.
L9	Front Royal	1040 Adams Ave.	Garden along S. side of private residence.

Table 6. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN SHENANDOAH VALLEY, VA --- TRIP 1

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks*
Front Royal	P1/L1	1040-1655	714	At 1040, T[a] = 21°C, RH[b] = 51%. Sky clear. No odor.
Front Royal	P1/L2	1115-1715	336	At 1115, T = 21°C, RH = 40%. Sky clear. No odor.
Front Royal	P1/L3	1140-1728	657	At 1140, T = 22°C, RH = 42%. Sky clear. Noticeable and unpleasant odor. Winds: S.W. at 1140.
Front Royal	P1/L4	1550-1345 (9/29 - 9/30)	22,900,000[c]	T = 6°C to 23°C. Wind: variable/calm to 1.7 m/s
Front Royal	P1/L4	1609-1305 (9/29 - 9/30)	228[d]	T = 6°C to 23°C. Wind: variable/calm to 1.7 m/s no clouds. Some odor.
Front Royal	P2/L3[e]	1735-0715 (9/29 - 9/30)	751[f]	T = 16°C to 19°C. Wind: variable; mostly S.W./calm to 1.4 m/s.
Front Royal	P2/L5[e]	2030-0635 (9/29 - 9/30)	567	T = 11°C to 6°C. Wind: variable/calm to 1.3 m/s. scattered clouds.
Front Royal	P3/L2	0737-1315	457	T = 12°C, RH = 82% at 0734. Sky clear. Heavy emissions and haze over Avtex.
Front Royal	P3/L3	0720-1300	576	T = 27°C, RH = 72% at 1305. Clear to partly cloudy.
Front Royal	P3/L6	0800-1325	325	T = 7°C to 20°C. Wind: variable/0.6 to 1.7 m/s. Faint odor.

[a] Temperature
[b] Relative humidity
[c] Sample collected with MAS
[d] Long-term sample collected with duPont personal sampling pump.
[e] Period 4 was an overnight sampling at two locations to sample potential nighttime emissions and/or settling due to atmospheric inversion.
[f] Pump malfunction during sampling period.

* General weather conditions for 9/29 and 9/30: Warm, skies clear to scattered clouds. No precipitation, slight winds.
Dates: 9/29-30/77

Table 7. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN SHENANDOAH VALLEY, VA --- Trip 2

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks
Front Royal	P1/L1	1508-2150	397	At 1510, T[a]= 19°C, RH[b]= 95%, overcast, no odor. Wind: N.N.W. to variable/0.8 m/s to calm. T = 19°C[e], RH = 87% to 90%[e].
Front Royal	P1/L2	1455-2115	411	At 1605, T = 20°C, RH = 85%, low ceiling, light drizzle. Slight odor. Wind: N.N.W. to variable/0.8 m/s to calm.
Front Royal	P1/L3	1520-2120	474	At 1600, T = 20°C, RH = 85%, low ceiling. Mild odor. Wind: N.N.W. to variable/0.8 m/s to calm.
Front Royal	P1/L4	1550-0850 (10/27-10/28)	183[c]	At 1550, T = 19°C, RH = 90%, overcast. No odor. Wind: N.N.W. to S.S.W./calm to 1.0 m/s.
Front Royal	P1/L5	1925-2315	457	Wind: variable/calm. T = 19 to 18°C[e], RH = 87% to 90%[e].
Front Royal	P2/L1	2155-0520	383[d]	Wind: variable to S.S.W./calm to 1 m/s. T = 19 to 17°C[e], RH = 87% to 90%[e].
Front Royal	P2/L2	2115-0555	666	Wind: variable to S.S.W./calm to 1 m/s. At 0555, strong odor. T = 19 to 16°C[e], RH = 87% to 90%[e].
Front Royal	P2/L3	2126-0620	705	Wind: variable to S.W.W./calm to 1 m/s. At 0620, no odor noticeable. T = 19 to 16°C[e], RH= 87% to 93%[e].
Front Royal	P2/L5	2330-0645	854	Wind: variable to S.S.W./calm to 1 m/s. Much auto exhaust, diesel fumes. T = 19 to 15°C[e], RH = 87% to 93%[e].

[a] Temperature

[b] Relative humidity

[c] Long-term sample collected with duPont personal sampling pump.

[d] Pump malfunctioned during sampling period.

[e] Data from National Weather Service Office, Dulles International Airport, Washington, DC.

[*] General weather conditions for 10/27 and 10/28: Moderate temperatures with high relative humidities after several days of steady rain. Winds generally calm with skies overcast and low cloud cover.

Dates: 10/27-28/77.

Table 8. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN SHENANDOAH VALLEY, VA --- TRIP 3

Site	Period/Location	Sampling Time	Sampling Volume (ℓ)	Remarks*
Front Royal	P1/L2	1540-2315	814	At 1545, T[a] = 8°C, RH[b] = 59%, wind: N/E~ 2 ms.
Front Royal	P1/L4	1330-0925 (11/14-11/16)	46,300,000[c]	T[a] = 4 to 15°C[e], RH[b] = 37% to 82%[e], winds: E.S.E. to S.S.W.[e]/calm to 7 m/s[e].
Front Royal	P1/L4	1315-0845 (11/14-11/16)	470[d]	At 0845 (11-16), scattered clouds, no odor. Winds: S.S.W. to E.S.E./calm to 7 m/s[e]. T[a]= -4 to 15°C[e], RH[b]= 37% to 82%[e].
Front Royal	P1/L7	1605-2330	1037	At 1600, strong odor apparently from Avtex. At 2330, wind calm, no odor. Winds: S.W.W. to S.S.E./ 2 to 3 m/s[e]. T[a] = 7 to 5°C[e], RH = 37% to 60%[e].
Front Royal	P1/L8	1637-2335	639	At 2335, wind calm, no odor. Winds: S.S.W. to S.S.E./ 2 to 3 m/s[e]. T= 7 to 5°C[e], RH = 37% to 60%[e].
Front Royal	P1/L9	1700-2345	731	At 1700, slight odor. At 2345, no odor. Winds: S.S.W. to S.S.E./ 2 to 3 m/s[e]. T = 7 to 5°C[e], RH = 37%-60%[e].
Front Royal	P2/L2	1000-1722	535	At 1000, overcast, no odor. T = 6 to 14°C[e], RH = 56% to 42%[e], Winds: S. to S.S.W.[e]/3 to 4 m/s[e].
Front Royal	P2/L7	1047-1705	1125	At 1047, slight odor. At 1705, no odor. T = 6 to 14°C[e] RH = 56% to 42%[e]. Winds: S. to S.S.W.[e]/3 to 4 m/s[e].
Front Royal	P2/L8	1015-1715	478	At 1015, overcast, strong odor. T = 6 to 14°C[e], RH = 56% to 42%[e]. Winds: S. to S.S.W.[e]/3 to 4 m/s[e].
Front Royal	P2/L9	1030-1710	1192	At 1030, odor of cooked apple. At 1710, no odor. T = 6 to 14°C[e], RH = 56% to 42%[e]. Winds: S. to S.S.W.[e]/ 3 to 4 m/s[e].

[a] Temperature.
[b] Relative humidity.
[c] Sample collected with MAS.
[d] Long-term sample collected with duPont personal sampling pump.
[e] Data from National Weather Service Office, Dulles International Airport, Washington, DC.

*General weather conditions for 11/14 through 11/16: Cool with clear to partly cloudy skies. Winds calm to brisk with occasional gusts.

Dates: 11/14-16/77.

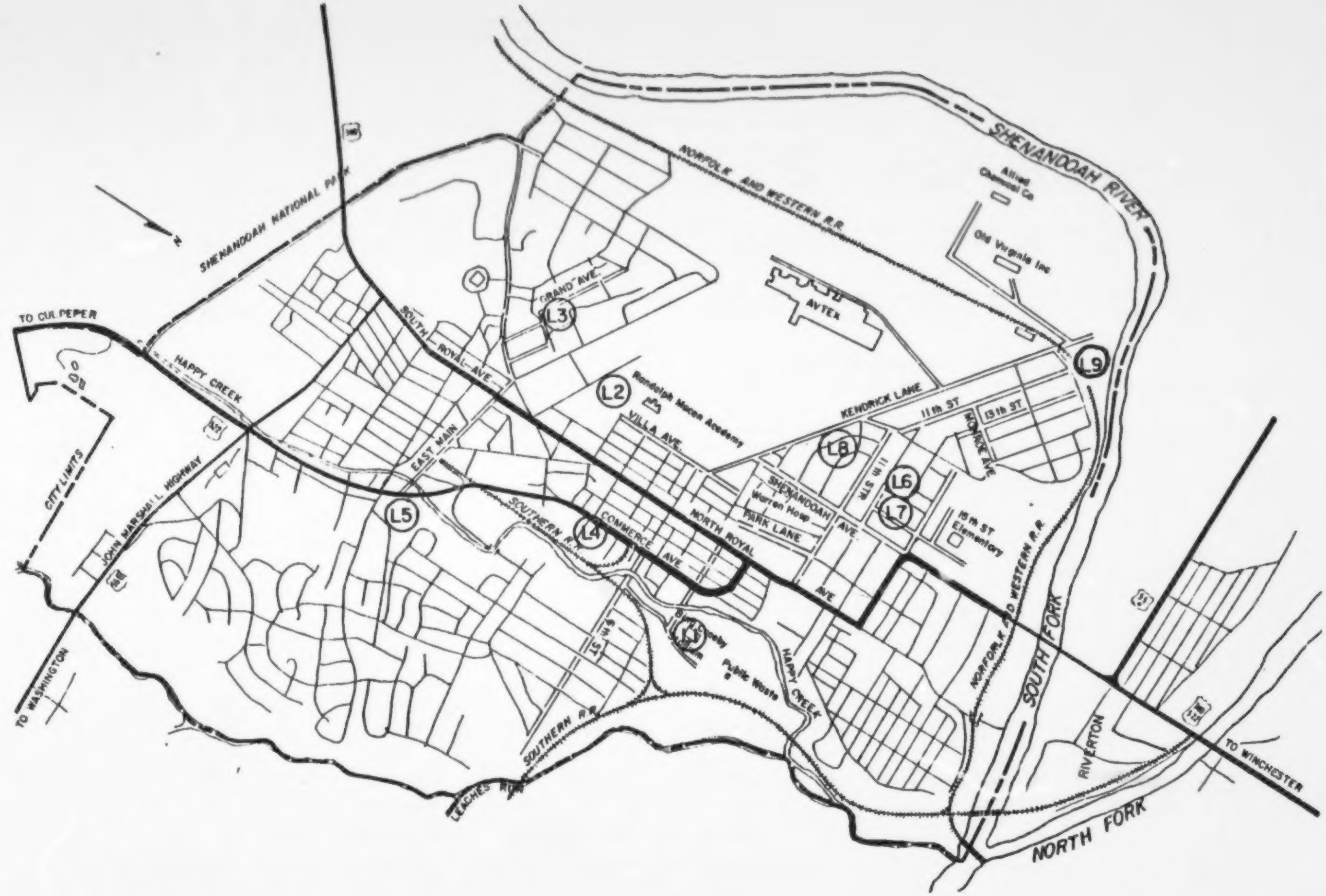

SHENANDOAH RIVER
Allied Chemical Co
Old Virginia Inc
NORFOLK AND WESTERN R.R.
AVTEX
SHENANDOAH NATIONAL PARK
N
TO CULPEPER
HAPPY CREEK
CITY LIMITS
JOHN MARSHALL HIGHWAY
TO WASHINGTON
SOUTH ROYAL AVE
GRAND AVE
L3
L2
Randolph Macon Academy
VILLA AVE
KENDRICK LANE
11th ST
13th ST
MONROE AVE
L8
L6
L7
11th STR
SHENANDOAH AVE
Warren Hosp
PARK LANE
NORTH ROYAL AVE
15th ST Elementary
EAST MAIN
L5
L4
COMMERCE AVE
SOUTHERN R.R.
6th ST
L1
Public Waste
HAPPY CREEK
SOUTHERN R.R.
LEACHES RUN
NORFOLK AND WESTERN R.R.
SOUTH FORK
NORTH FORK
RIVERTON
L9
TO WINCHESTER
340
522
55

Figure 8. Map of Front Royal, VA showing sampling locations described in Table 5.

PARTICULATE COLLECTED WITH MAS

Table 9 summarizes the amounts of particulate scraped from the collection plates of the MAS. During the first trip to both locations the ionizing wires were broken and the collection of < 1.7 μ particulate was very poor. The second trip to Charleston resulted in low collection due to high humidity and occasional rain which forced operation of the sampler at a lower plate voltage (and concomitant lower collection efficiency). In addition, the rain scrubbed most of the particulate of interest out of the air. No particulate was collected on the second trip to Front Royal due to a steady rain throughout most of the sampling period. The rain not only scrubbed most of the particulate of interest from the air but also prevented operation of the MAS with any voltage supplied to the electrostatic precipitator plates due to excessive arcing. During the third trip to both Front Royal and Charleston, cool, dry weather permitted long collection periods at high plate voltages. These conditions allowed collection of more than one gram of < 1.7 μ particulate from both locations. Only the samples from Trip 3 were sufficient for GC/MS/COMP analysis.

Table 9. SUMMARY OF PARTICULATE SAMPLING WITH MAS FOR SHENANDOAH AND KANAWHA VALLEYS

Site	Trip No.	Volume of Air Sampled (ℓ)	Amount Collected (g)		
			> 3.5 μ	3.5 - 1.7 μ	< 1.7 μ
Charleston (P1/L1)	1	29,500,000	0.1587	0.0838	0.0035[a]
Charleston (P1/L1)	2	49,700,000	0.1653	0.1833	0.6364
Charleston (P1/L1)	3	90,800,000	0.2100	0.1552	1.8171
Front Royal (P1/L4)	1	22,900,000	0.0710	0.0391	0.2589[a]
Front Royal (P1/L4)	2	——— b	—	—	—
Front Royal (P1/L4)	3	46,300,000	0.0998	0.0558	1.1457

---

[a] Ionizing wires were not properly charged; therefore, the amounts collected were very low.
[b] No sample collected due to continuous rain and high humidity.

SECTION 6
SAMPLE ANALYSIS

ANALYSIS OF TENAX GC CARTRIDGES BY GC/MS/COMP

Air samples collected on Tenax GC cartridges were analyzed by capillary column GC/MS/COMP. The whole sample was introduced to the analytical system by thermal desorption into a cryogenic capillary trap and thence rapidly swept onto the chromatographic column. Each cartridge was loaded with a known amount of perfluorobenzene and perfluorotoluene for use in quantitation. Qualitative data interpretation was done by visual interpretation of the spectra and comparison with standard reference spectra. Quantitation was achieved by integration of a characteristic mass for a compound over the chromatographic peak. The amount of compound in the sample was then calculated using the relative molar response factor and the integrated area for a standard. The concentration in ambient air was then calculated using the volume sampled or the breakthrough volume, whichever was larger. Complete details of the sample analysis are in Appendix A.

ANALYSIS OF CARBON CARTRIDGES BY GC/MS/COMP

Carbon backup cartridges contained the very volatile compounds which have very low breakthrough volumes on Tenax GC (and thus would have high detection limits). The cartridges were not amenable to direct thermal desorption/analysis due to high background (notably water). However, the compounds of interest (methylene chloride, vinyl chloride, acetaldehyde, etc.) were eluted from the carbon cartridge at 270° onto a Tenax GC cartridge using helium. These Tenax GC transfer cartridges were then analyzed in the manner described for the Tenax GC cartridges collected in the field. This procedure was fully validated on previous contracts. Complete details of the sample analysis are in Appendix B.

ANALYSIS OF SEMIVOLATILE ORGANICS COLLECTED BY MAS SAMPLER

Extraction/Partition Scheme

Two extraction/partition schemes were used for extraction of the semivolatile organics from air particulate. The first scheme, used on the < 1.7 μ fraction collected in Charleston, WV during Trip 3, yielded six fractions. This extent of fractionation resulted in concentrations which were too low for effective GC/MS/COMP analysis. A second scheme, employed for the < 1.7 μ fraction for Front Royal, VA during Trip 3, resulted in two fractions and yielded much more concentrated samples. The GC/MS/COMP data from this sample were easier to interpret.

Analysis efforts were directed toward the < 1.7 μ fraction, as this size particle is the most easily lodged in the respiratory system and is therefore most significant with respect to potential human health effects. For reasons discussed in the Sampling Section, only the samples collected on Trip 3 were of sufficient volume to warrant extraction and analysis.

The <1.7 μ fraction, scraped from the electrostatic precipitator plate of the MAS, was extracted by repeated sonication with cyclohexane and then with methanol. The methanol was effective in removing the more polar compounds. The extracts were then combined and fractionated according to the scheme presented in Figure 9. The individual fractions were then concentrated for GC/MS/COMP analysis. This extraction scheme was developed under another contract.(13)

The efficacy of the scheme was assessed by subjecting a mixture containing known amounts of compounds to the partition procedure. The mixture consisted of benzoic acid, phenol, quinoline, hexadecane, phenanthrene and ethylene glycol. The compounds were chosen to represent the five classes of materials produced by the partition scheme (all these materials have been found in air particulate samples, except ethylene glycol). No information on the composition of the polar neutral fraction was available, therefore ethylene glycol was included as a likely component of this fraction based on its known chemical properties. The experiment was conducted using both large and small mass samples. Recoveries were determined gravimetrically.

As a further check on the procedure, thin layer chromatography (TLC) scans were conducted on each fraction to ascertain the extent, if any, of

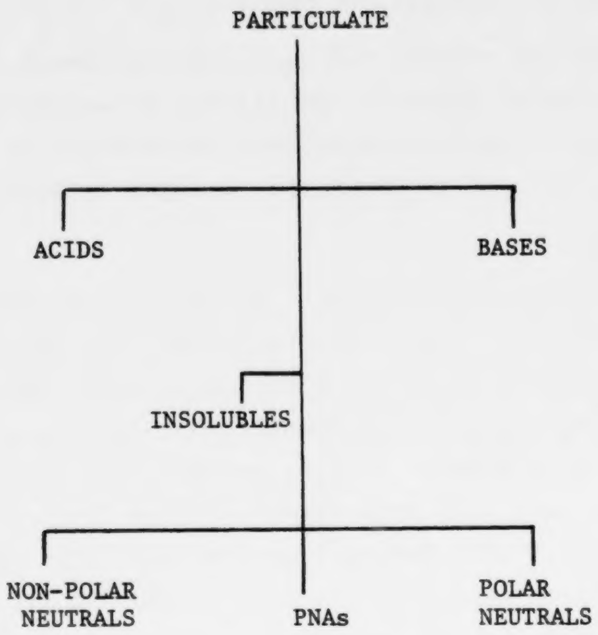

PARTICULATE
ACIDS
BASES
INSOLUBLES
NON-POLAR NEUTRALS
PNAs
POLAR NEUTRALS

Figure 9. Fractionation scheme used for fractionating air particulate collected in Charleston, WV (Trip 3, P1/L1).

compound spillover into other fraction(s). No such spillover was detected.

Scheme Used for Front Royal, VA Sample --

The sample was weighed, 102 µg d_{10}-pyrene (Merck & Co., Rahway, NY) added as an internal standard, and allowed to equilibrate overnight. The sample was then extracted with toluene and methanol as shown in Figure 10. The two fractions thus generated were analyzed by GC/MS/COMP.

GC/MS/COMP Analysis

Samples were analyzed using a LKB 2091 gas chromatograph/mass spectrometer with a dedicated PDP-11/34 data system. The samples were chromatographed on an OV-101 capillary column (25 m, WCOT, obtained from LKB). The column was held at 100°C for 2 minutes after injection, and then heated to 265°C at a rate of 8°/min. Carrier gas flow rate was 2.0 ml/min with a split ratio of 10:1. Injector temperature was 240°C. Mass spectral scans were taken every 3 sec scanning from 5-492 amu. The ion source temperature was 200°; electron energy, 70 eV; trap current, 50 µA; accelerating voltage, 3500 V; and multiplier setting 425-450. Total ion current and mass spectra plots were generated for interpretation.

Data were interpreted by comparison of the unknown spectra with standard reference collections. Where no reference spectrum was available, or where spectral quality was not sufficient for positive identification, the compounds were labeled "tentative." All interpretations were made independently by two chemists and then correlated. Further validation of equivocal identifications was made by consultation with other chemists and spectroscopists experienced in similar research. This mass spectral interpretation protocol was established to extract the maximum information from the data and to guard against misidentification. Quantitation of the compounds identified in the semivolatile fractions was not feasible due to a lack of available standards to generate relative molar response factors. Rough quantitation may be made by comparison of peak heights on the total ion current chromatograms.

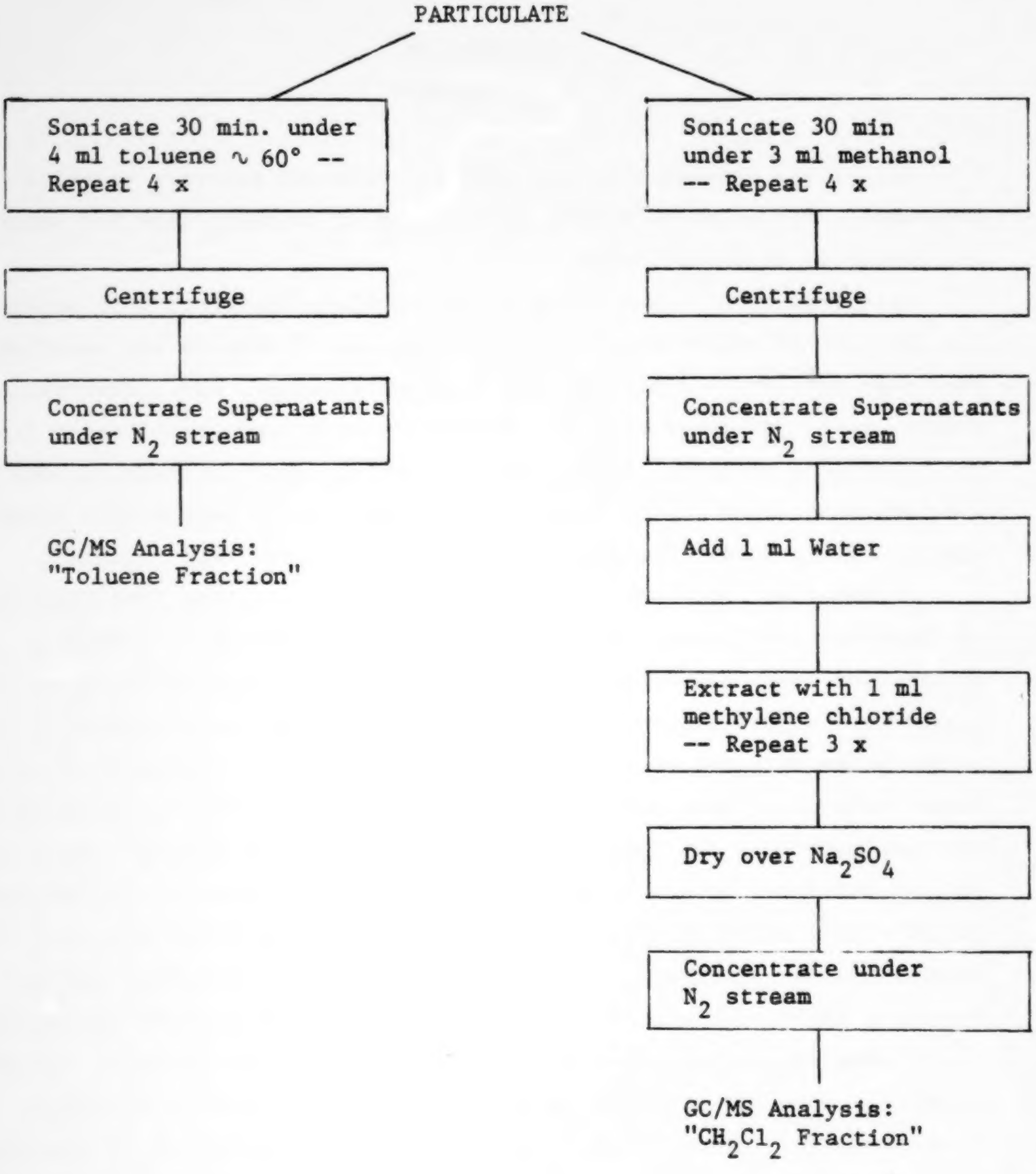

PARTICULATE
Sonicate 30 min. under 4 ml toluene ∿ 60° -- Repeat 4 x
Centrifuge
Concentrate Supernatants under N_2 stream
GC/MS Analysis: "Toluene Fraction"
Sonicate 30 min under 3 ml methanol -- Repeat 4 x
Centrifuge
Concentrate Supernatants under N_2 stream
Add 1 ml Water
Extract with 1 ml methylene chloride -- Repeat 3 x
Dry over Na_2SO_4
Concentrate under N_2 stream
GC/MS Analysis: "CH_2Cl_2 Fraction"

Figure 10. Extraction scheme used for fractionating air particulate collected in Front Royal, VA.

SECTION 7

RESULTS

All of the samples were analyzed for volatile and very volatile compounds. The GC/MS/COMP data were stored on magnetic tape for subsequent processing as discussed below.

Data from about one-quarter of the sampling locations were selected for qualitative interpretation. The selection of samples was based on knowledge obtained during sampling (e.g. meteorology, odor, observation of plumes, etc.) and inspection of the total ion current chromatogram from the GC/MS/COMP analysis. Only selected samples were interpreted because the compounds found in the area are not likely to be unique to a particular sample. Thus, interpretation of all data would have been redundant.

A number of compounds were selected for quantitation from the lists of compounds identified. Quantitation was performed on all samples. All halogenated compounds found were quantitated and only representative compounds from other classes were quantitated. The values presented in the tables below were not corrected for recoveries. The recoveries of standards loaded onto cartridges are presented in Table 11. Since recovery corrections were not made, all concentrations must be regarded as minima. Where trace (not quantitated) levels were observed, the designation "T" is followed by the detection limit in parentheses. Where no compound was observed, the detection limit is shown. The detection limits varied widely and were dependent upon the breakthrough volume (which is temperature-dependent), volume sampled, and relative molar response, as discussed above. As these parameters were not constant among the samples, the detection limits varied widely. In some cases compounds were identifed in the qualitative analysis scheme, but were reported below the detection limit in the quantitation. This is due to the threshold set during the quantitation to prevent noise from being quantitated and reported. Thus, trace quantities which were observed in the qualitative data interpretation were not detected during quantitation. These samples may be regarded as trace.

Table 10. RECOVERIES OF SELECTED ORGANIC VAPORS FROM TENAX CARTRIDGES SUBJECTED TO SAMPLE TRANSPORTATION AND STORAGE

Trip No.	Chemical	Quantity Added (ng)	Quantity Observed (ng)	% Recovery
1	methylene chloride	325	260	80
	chloroform	197	108	55
	1,1,1-trichloroethane	35	24	69
	benzene	249	234	93
	toluene	112	117	104
2	methylene chloride	300	218	72
	chloroform	200	109	55
	1,1,1-trichloroethane	35	20	57
	benzene	241	268	111
	toluene	110	77	70

ORGANIC COMPOUNDS IN THE KANAWHA VALLEY, WV

Volatile Organics

The volatile compounds identified on Tenax GC and/or carbon cartridges at ten locations are presented in Table 11. Alkanes and alkenes were generally not listed in the summary tables due to their ubiquity and relatively benign environmental effects. Full lists of the compounds found in each sample are contained in Appendix C. The quantitative results for the halogenated hydrocarbons and representative compounds in other chemical classes are presented in Tables 12-14 and 15-17, respectively.

Halogenated Hydrocarbons--

The levels of halogenated hydrocarbons in the Kanawha Valley during the first trip were generally low. Significantly higher levels were observed on the second trip, especially in South Charleston (P2/L2). During the third trip, significant levels of some compounds were observed at several sites, including S. Charleston (P3/L2) Charleston (P1/L1), and Institute (P2/L8).

Trichloroethylene concentrations at L4 were consistently higher than at other locations. Similarly, higher concentrations of tetrachlorethylene were observed occasionally in South Charleston (L2). High levels of chloroform, methylene chloride, and carbon tetrachloride did not seem to be correlated to any specific location and were often independent of each other.

Volatile Organics - (Non-halogenated)--

As with the halogenated compounds, the organic concentrations during the first trip were generally low. Very high concentrations were observed during the second trip in St. Albans and, to a lesser extent in S. Charleston. Moderately high levels of some compounds were observed in Institute during both sampling periods of Trip 3.

As expected, the levels of aromatics (benzene, toluene, and naphthalene) show a loose general correlation. The acetophenone level on Trip 3, P2/L2 was more than ten times higher than any other observed level. Similarly, the ethyl acetate level on Trip 2, P2/L3 was 30 times higher than in any other sample.

Table 11. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
HALOGENATED										
Vinylidene chloride and/or dichloroethylene isomer	T[d]	+	+	-	-	+	+	+	+	+
Methylene chloride	+	+	+	+	+	+	+	+	+	+
Chloroform	+	+	+	+	+	+	+	+	+	+
1,2-Dichloroethane	T	-	-	T	-	-	-	-	-	-
1,1,1-Trichloroethane	+	+	+	+	+	-	+	+	+	-
1-Chlorobutane	-	-	-	-	+	-	-	-	-	-
Carbon tetrachloride	+	+	-	+	+	+	+	+	+	-
Dichloropropene	-	-	-	-	+	-	-	-	-	-
Trichloroethylene	+	T	T	+	+	-	-	-	+	-
1,2-Dibromoethane	-	-	-	T	T	-	-	-	-	-
Tetrachloroethylene	+	+	+	+	+	T	+	+	+	-
Chlorobenzene	-	-	-	-	-	-	+	-	-	-
Dichlorobenzene	+	+	T	+	+	-	+	+	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
ALDEHYDES										
Acetaldehyde	+	+	+	+	T	+	+	+	+	-
2-Methylpropanal	-	-	-	+	+	-	-	-	-	-
n-Butanal	T	-	+	-	-	-	T	-	+	-
n-Pentanal	+	-	-	-	-	-	-	-	-	-
2-Ethylbutanal	-	-	-	+	-	-	-	-	-	-
n-Hexanal	-	T	-	-	-	+	-	-	+	-
Dimethylpentanal	-	-	-	-	+	-	-	-	-	-
n-Heptanal	T	-	-	+	-	+	-	-	-	-
Benzaldehyde	+	+	+	+	+	+	+	+	+	-
n-Octanal	T	+	+	-	-	+	-	-	+	-
n-Nonanal	-	+	+	-	-	+	+	+	+	-
n-Decanal	-	+	-	-	-	+	-	+	-	-
n-Undecanal	-	T	-	-	-	+	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
KETONES										
Acetone	+	+	+	+	+	+	+	+	+	+
Methyl isopropyl ketone	+	-	-	T	-	-	-	-	-	-
Methyl vinyl ketone	T	-	-	-	-	-	-	-	-	-
Methyl ethyl ketone	-	-	+	+	T	-	T	-	-	-
3-Penanone	-	-	-	+	-	-	-	-	-	-
4-Methyl-2-pentanone	+	-	-	+	+	-	+	-	-	-
$C_6H_{10}O$ isomer	-	-	-	-	-	-	T	-	-	-
$C_6H_{12}O$ isomer	-	-	-	-	-	-	T	-	+	-
4-Methyl-3-penten-2-one	-	-	-	-	-	-	+	-	-	-
$C_7H_{14}O$ isomer	-	-	-	T	-	-	-	-	-	-
Heptanone	-	-	-	-	-	-	+	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
KETONES (continued)										
$C_9H_{18}O$ isomer	-	-	-	-	-	-	+	-	-	-
Acetophenone	+	+	+	-	-	+	+	+	T	-
3,5,5-Trimethyl-2-cyclohexenone	-	-	-	-	-	-	+	-	-	-
2-Pyrone	-	-	-	-	-	-	T	-	-	-
$C_{10}H_{20}O$ isomer	-	-	-	-	-	-	-	+	-	-
2,6,8-Trimethylnonanone	-	-	-	-	-	-	+	-	-	-
$C_{12}H_{24}O$ isomer	-	-	-	-	-	-	T	-	-	-
$C_{10}H_{10}O$ ketone isomer	-	-	-	-	+	-	-	-	-	-
α-Tetralone	-	-	-	-	-	-	+	-	-	-
1,2,3,4-Tetrahydronaphthalene-1-one	-	-	-	-	-	-	-	-	+	-
Alkyl ketone	-	-	-	-	-	-	-	-	+	
Benzophenone	-	-	-	-	+	-	+	+	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
ESTERS										
Methyl formate	-	-	-	T	-	-	-	-	-	-
Methyl acetate	-	-	-	+	+	-	T	-	-	-
Ethyl acetate	-	+	+	+	T	T	-	+	-	-
Isopropyl acetate	-	-	-	+	T	-	-	-	-	-
Isopropenyl acetate	-	-	-	+	-	-	-	-	-	-
n-Propyl acetate	-	-	-	+	+	-	-	-	-	-
n-Butyl acetate	-	-	-	+	-	-	-	-	-	+
C_6H_{11} acetate	-	-	-	+	-	-	-	-	-	-
ALCOHOLS										
Isopropanol	-	-	-	T	+	-	-	-	-	-
2-Hexanol	-	-	-	-	-	-	+	-	-	-
Alcohol isomer	-	-	-	T	-	-	-	-	-	-
Phenol	+	+	-	T	-	+	+	+	T	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
ALCOHOLS (continued)										
Cresol	-	-	-	-	-	+	-	-	-	-
Dimethylphenol isomer	-	-	-	-	-	+	-	-	-	-
C_2-alkyl phenol	+	+	T	+	+	+	-	+	-	-
C_3-alkyl phenol	-	+	-	-	-	+	-	-	-	-
ETHERS										
Dimethyl ether	-	+	+	T	-	+	+	-	-	-
Diethyl ether	-	+	+	-	-	-	-	+	T	+
Furan	T	-	-	T	-	-	-	-	T	-
Diisopropyl ether	-	-	-	+	+	+	+	-	-	-
Alkyl ether	-	-	-	T	-	-	-	-	-	-
Alkyl ether	-	-	-	-	-	-	+	-	-	-
2-Methoxy-2h-dihydro-pyran	-	-	-	-	-	-	+	-	-	-
Anisole	-	-	-	-	+	-	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
ETHERS (continued)										
Benzofuran	-	-	-	-	-	-	+	-	-	-
Diphenyl ether	+	T	-	-	+	-	+	-	-	-
AROMATICS										
Benzene	+	+	+	+	+	+	+	+	+	-
Toluene	+	+	+	+	+	+	+	+	+	-
Ethylbenzene	+	+	+	+	+	+	+	+	+	-
Styrene	+	+	+	+	+	+	+	+	+	-
Xylene	+	+	+	+	+	+	+	+	+	-
Propylbenzene	+	+	+	+	+	+	+	+	+	-
Ethyltoluene	+	+	+	+	+	+	+	+	+	-
Trimethylbenzene	+	+	+	+	+	+	+	+	+	-
o-Ethyltoluene	+	+	+	+	+	-	+	+	+	-
C_3H_5 benzene	-	-	-	+	+	-	-	+	+	-
C_3-alkylbenzene	-	-	-	+	-	+	-	+	-	-
Methylstyrene isomer	-	-	T	-	-	-	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
AROMATICS (continued)										
C_4-alkylbenzene	+	+	+	+	+	+	+	+	+	-
i-Butylbenzene	-	-	-	+	-	-	-	-	+	-
sec-Butylbenzene	-	-	-	+	-	-	-	-	+	-
Indan	+	+	+	+	+	-	+	+	-	-
Indene	-	-	-	-	-	-	+	-	-	-
n-Butylbenzene	-	-	+	-	+	-	-	-	-	-
Propyltoluene	-	-	-	+	-	-	-	-	+	-
C_5-alkylbenzene	+	+	+	+	+	-	+	+	+	-
Tetramethylbenzene	-	-	-	+	+	-	-	-	+	-
1,2,3,4-Tetrahydronaphthalene	+	-	-	+	+	-	+	-	+	-
C_4H_7 benzene isomer	-	+	-	+	+	-	+	+	+	-
Naphthalene	+	+	+	+	+	-	+	+	+	-
Methyldihydronaphthalene	-	-	-	-	-	-	T	-	-	-
C_5H_9 benzene isomer	+	-	-	+	-	-	-	-	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
AROMATICS (continued)										
C_6-alkylbenzene	+	–	–	+	+	–	–	–	+	–
β-Methylnaphthalene	+	+	+	+	+	+	+	+	+	–
α-Methylnaphthalene	+	+	+	+	+	–	+	+	+	–
C_6H_{11} benzene	–	–	–	–	T	–	–	–	–	–
C_7-Alkylbenzene	–	–	–	–	+	–	–	–	–	–
C_2-Alkylnaphthalene	–	T	+	+	–	–	+	+	–	–
Dimethylnaphthalene isomer	+	–	–	+	+	–	–	+	+	–
Biphenyl	+	+	–	+	+	T	+	–	+	–
C_3-Alkylnaphthalene	–	–	–	+	+	–	–	–	–	–
SULFUR CONTAINING										
CS_2	+	+	+	+	+	–	–	–	–	+
Dimethyl disulfide	–	–	–	–	+	–	–	–	–	–
2,3-Benzothiophene	–	–	–	–	–	–	T	–	–	–

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2				Trip 3		
	P2/L2[a]	P2/L5[a]	P2/L6[a]	P2/L3[b]	P2/L4[b]	P2/L5[b]	P1/L8[a]	P2/L1[b]	P2/L2[b]	P2/L9[c]
NITROGEN CONTAINING										
Cyanobenzene	-	-	-	-	-	-	+	-	-	-
C_3-alkyl pyridine	-	-	-	-	-	-	T	-	-	-
MISCELLANEOUS										
Butene	-	+	+	-	-	-	-	-	-	-
4-Vinylcyclohexene	-	-	-	-	+	-	-	-	-	-

Notes

[a] Both Tenax GC and carbon cartridge samples interpreted

[b] Tenax GC cartridge sample interpreted

[c] Carbon cartridge sample interpreted

[d] + = identified
- = not identified
T = tentative identification

[alkanes, alkenes, and artifacts not included]

Table 12. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV --- TRIP 1.

Chemical	Period/Location								
	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L5	P2/L6
methylene chloride	T(1000)	T(1000)	T(714)	T(714)	<625	T(555)	778	<555	<555
chloroform	T(167)	T(167)	T(125)	T(125)	<120	T(97)	T(97)	<97	<97
carbon tetrachloride	<625	T(125)	<95	T(95)	<91	T(74)	T(74)	<74	<74
vinyl chloride	<15000	<12000	<12000	<12000	<10000	<10000	<10000	<10000	<10000
1,2-dichloroethylene	<545	<334	T(334)	<334	T(322)	<322	T(322)	<263	<263
1,1-dichloroethane	<380	<286	<285	<285	<345	<345	<345	<228	<228
1,2-dichloroethane	T(347)	T(258)	<258	<258	T(250)	<256	<256	<195	<195
1,1,1-trichloroethane	T(417)	T(334)	T(334)	T(334)	T(312)	T(312)	T(312)	<278	<278
1,1,2-trichloroethane	<294	<250	<250	<250	<238	-	<217	<218	<218
trichloroethylene	T(132)	T(100)	<100	300	<98	T(98)	T(98)	<74	<74
tetrachloroethylene	T(48)	T(35)	T(36)	<36	T(36)	146	T(26)	<26	<26
1,1,1,2-tetrachloroethane	<23	<31	<31	<31	<30	<30	<30	<22	<22
1,1,2,2-tetrachloroethane	<23	<31	<31	<31	<30	<30	<30	<22	<22
pentachloroethane	<13	<8	<9	<10	<9	<9	<9	<9	<12
hexachloroethane	<13	<8	<9	<10	<9	<9	<9	<9	<12
chlorobenzene	<58	<25	<27	T(32)	<32	<32	<32	<27	<36
o-dichlorobenzene	<39	T(17)	<18	<20	<18	T(18)	<18	<18	<24
m-dichlorobenzene	<39	T(28)	T(18)	T(20)	T(18)	38	<14	<18	<24
p-dichlorobenzene	<35	<15	<16	<18	<16	<16	-	<17	<30
1,2,4-trichlorobenzene	<23	<10	<11	<12	<11	<11	<8	<11	<15
1,3,5-trichlorobenzene	<13	<8	<9	<10	<9	<9	<7	<9	<12
1,2,3-trichlorobenzene	<23	<10	<11	<12	<11	<11	<8	<11	<15
vinylidene chloride	<454	<334	<334	<334	<345	<345	<345	<263	<263

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

Table 13. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV --- TRIP 2.

	Period/Location									
Chemical	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L4	P2/L5	B
methylene chloride	867	715	T(714)	T(714)	T(714)	11334	T(555)	T(555)	1778	≤7
chloroform	177	T(125)	T(125)	T(125)	T(125)	2161	161	1333	T(97)	≤3
carbon tetrachloride	215	T(95)	T(95)	T(95)	T(95)	2222	3630	97	T(74)	≤2
vinyl chloride	<10000	<12000	<12000	<12000	<12000	<10000	<10000	<10000	<10000	<15
1,2-dichloroethylene	T(263)	<334	<334	T(334)	T(334)	T(263)	<263	<263	T(263)	≤10
1,1-dichloroethane	<228	<228	<228	<228	<228	<228	<228	<228	<228	<8
1,2-dichloroethane	T(195)	T(258)	<258	T(258)	<258	T(195)	T(195)	T(195)	T(195)	≤8
1,1,1-trichloroethane	278	T(334)	T(334)	T(334)	T(334)	3278	T(278)	T(278)	<278	≤5
1,1,2-trichloroethane	<217	<250	<250	<250	<250	<217	<217	<217	<217	<5
trichloroethylene	<74	<100	<100	360	T(100)	179	45	358	T(75)	≤5
tetrachloroethylene	109	T(36)	<36	T(360)	T(36)	1536	434	52	<26	<7
1,1,1,2-tetrachloroethane	<22	<31	<31	<31	<31	<20	<22	<22	<22	<6
1,1,2,2-tetrachloroethane	<22	<31	<31	<31	<31	<20	<22	<22	<22	<6
pentachloroethane	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5
hexachloroethane	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5
chlorobenzene	T(29)	T(56)	<40	<40	T(36)	44	<35	T(37)	<26	<15
o-dichlorobenzene	<19	T(37)	<27	T(27)	<24	306	T(23)	39	<17	<10
m-dichlorobenzene	101	T(37)	<27	T(27)	T(24)	276	T(23)	T(24)	<17	<10
p-dichlorobenzene	<18	<34	<24	<24	<22	T(33)	<21	<22	<16	<9
1,2,4-trichlorobenzene	<12	<22	<16	<16	<14	<20	<14	<15	<12	<6
1,3,5-trichlorobenzene	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5
1,2,3-trichlorobenzene	<12	<22	<16	<16	<14	<20	<14	<15	<12	<6
vinylidene chloride	T(263)	<334	<334	<334	<334	<263	<263	<263	<263	<10

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

Table 14. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV --- TRIP 3

Chemical	Period/Location									
	P1/L1	P2/L2	P2/L5	P2/L7	P2/L8	P3/L1	P3/L2	P3/L5	P3/L8	P3/L9
methylene chloride	2818	T(454)	T(454)	T(454)	4091	1636	9818	1272	1636	1600
chloroform	428	T(71)	T(71)	T(71)	333	T(71)	262	T(71)	T(71)	T(71)
carbon tetrachloride	529	T(59)	T(59)	T(59)	441	T(59)	500	T(59)	T(59)	T(59)
vinyl chloride	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500
1,2-dichloroethylene	T(212)	T(213)	T(212)	T(213)	T(213)	T(213)	T(213)	<213	<213	T(213)
1,1-dichloroethane	<160	<160	<160	<160	<160	<160	<160	<160	<160	<160
1,2-dichloroethane	T(151)	151	T(163)	T(151)	T(151)	T(151)	T(151)	T(151)	T(151)	T(151)
1,1,1-trichloroethane	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	347	T(217)
1,1,2-trichloroethane	<167	<167	<94	<167	<167	<167	<167	<167	<167	<167
trichloroethylene	T(56)	T(56)	T(55)	T(55)	T(55)	T(55)	T(55)	T(55)	T(55)	<144
tetrachloroethylene	T(20)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)
pentachloroethane	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6
hexachloroethane	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6
chlorobenzene	<44	<17	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)
o-dichlorobenzene	<29	<9	T(8)	T(12)	59	<9	T(9)	T(9)	T(9)	T(9)
m-dichlorobenzene	<29	<16	T(8)	T(12)	T(12)	<18	<9	T(9)	T(9)	T(9)
p-dichlorobenzene	<26	<8	<7	<7	<7	<7	<7	<7	<7	<7
1,2,4-trichlorobenzene	<17	<6	<7	<7	<7	<7	<7	<7	<7	<7
1,3,5-trichlorobenzene	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6
1,2,3-trichlorobenzene	<17	<6	<7	<7	<7	<7	<7	<7	<7	<7
vinylidene chloride	<212	<213	<212	<213	<213	<213	<213	<213	<213	<213
1,1,1,2-tetrachloroethane	<17	<16	<17	<16	<16	<16	<16	<16	<16	<16
1,1,2,2-tetrachloroethane	<17	<16	<17	<16	<16	<16	<16	<16	<16	<16

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

Table 15. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV --- TRIP 1.

Chemical	Period/Location									
	B	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L5	P2/L6
benzene	≤3	259	117	44	28	69	36	83	102	120
toluene	≤3	178	212	27	115	83	518	95	297	310
naphthalene	≤3	31	55	9	17	13	57	8	24	32
acetophenone	≤10	T(39)	80	<18	78	41	217	<14	54	124
n-octanal	≤10	T(39)	11	18	T(20)	T(18)	T(22)	T(18)	T(2)	T(30)
benzophenone	≤10	T(39)	T(17)	T(18)	T(20)	T(18)	T(18)	T(14)	<18	<24
phenol	≤15	T(58)	16	20	T(30)	13	T(27)	<21	13	T(37)
diphenyl ether	<10	<39	<17	T(18)	T(20)	<18	<18	<14	T(18)	<24
ethyl acetate	<7	<43	T(43)	<43	<43	<43	T(97)	T(31)	<43	T(43)
cyanobenzene	<5	T(15)	10	6	T(10)	<9	20	<7	<9	<12
dimethyldisulfide	<8	<77	<77	<77	68	<77	163	<77	<77	<77

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

B = blank control. Values are in ng/cartridge.

Table 16. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV ---TRIP 2

	Period/Location									
	P1/L6	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L4	P2/L5	B
benzene	1611	259	203	185	389	3444	71778	296	593	<3
toluene	1441	93	144	241	192	1297	2865	906	392	<3
naphthalene	87	T(7)	29	34	13	3758	4694	321	23	<3
acetophenone	195	173	168	740	136	4950	<23	24	91	<10
n-octanal	<29	T(22)	<22	1044	T(44)	167	<22	24	T(22)	<10
benzophenone	T(29)	48	<22	<21	<22	374	<23	T(24)	22	<10
phenol	T(44)	20	<36	32	24	415	743	36	42	<15
diphenyl ether	<29	<25	<22	<21	<22	T(34)	208	T(24)	T(18)	<10
ethyl acetate	T(43)	T(97)	<97	T(97)	T(97)	91	6917	97	208	<7
cyanobenzene	24	<12	<12	<10	11	<17	<35	<12	<8	<5
dimethyldisulfide	<77	<163	<163	<163	<163	489	489	388	<489	<8

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.
B = blank control. Values are in ng/cartridge.

Table 17. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE KANAWHA VALLEY, WV --- TRIP 3

Chemical	Period/Location									
	P1/L1	P2/L2	P2/L5	P2/L7	P2/L8	P3/L1	P3/L2	P3/L5	P3/L8	P3/L9
benzene	334	555	305	778	2185	667	315	667	2287	250
toluene	53	449	111	<103	714	654	502	452	152	295
naphthalene	29	111	11	108	80	87	73	28	280	19
acetophenone	93	143	71	171	319	195	317	62	132	63
n-octanal	T(29)	25	T(18)	T(14)	T(18)	<29	<18	<18	14	345
benzophenone	<29	<9	<8	<21	T(12)	T(29)	46	T(9)	T(13)	10
phenol	20	8	11	38	42	T(44)	6	T(14)	10	T(15)
diphenyl ether	<29	<9	<8	<21	T(12)	<29	<16	<9	T(13)	T(10)
ethyl acetate	T(43)	T(43)	T(43)	T(43)	83	T(43)	T(43)	43	49	T(43)
cyanobenzene	T(14)	20	15	35	45	24	11	10	12	T(8)
dimethyldisulfide	<77	<77	<77	<77	<77	<77	<77	<77	<77	T(77)

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

Correlation between Levels of Halogenated and Non-halogenated Organics --

There are no general correlation between the levels of halogenated and non-halogenated organics in the Kanawha Valley. Two samples (Trip 2, P2/L2 and P2/L3) contained high levels of both halogenated and non-halogenated compounds.

Semivolatiles

The compounds identified in the polar neutral, PNA, paraffin and base fractions of the <1.7 μ air particulate are shown in Appendix D. The few compounds identified in the acid fraction were contained in other fractions also. It should be noted that the computer scales the TIC plot to the largest peaks. Therefore quantitative comparisons between fractions are not possible.

ORGANIC COMPOUNDS IN THE SHENANDOAH VALLEY, VA

Volatile Organics

A summary of the volatile compounds identified on Tenax GC and/or carbon cartridges at nine locations are presented in Table 18. Alkanes and alkenes were generally not summarized because of their ubiquity and relatively benign environmental effects. Full lists of the compounds found in each sample are contained in Appendix E. The quantitation results for the halogenated hydrocarbons and representative compounds in other chemical classes are presented in Tables 19-21 and 22-24, respectively.

The highest concentrations of volatile organics found on Trip 1 was at P2/L3 and P2/L5 which were night samples. P2/L3 was downwind of the Avtex plant at least part of the sampling period. The other samples obtained on this trip contained moderate amounts of volatile organics. The samples collected during Trip 2 contained high amounts of volatile compounds. The highest concentrations were again in the overnight samples (P1/L4, P2/L3, and P2/L5). L4 and L5 were in the downtown Front Royal area, which was in the floor of the valley. Thus, settling of pollutants in the lower areas during a night-time atmospheric inversion may have contributed to these high values. The other location (L3), however, was on top of a hill, so atmospheric inversion conditions would not explain high values at this point. The values obtained for P1/L3 were also relatively high. This sample was collected during the late afternoon-evening, so some of the

Table 18. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR IN THE SHENANDOAH VALLEY, VA (FRONT ROYAL)

CHEMICAL CLASS	Period/Location								
	Trip 1				Trip 2		Trip 3		
	P1/L4[a]	P2/L5[a]	P3/L2[b]	P3/L6[c]	P2/L3[b]	P3/L5[b]	P1/L9[a]	P2/L8[b]	P2/L9[b]
HALOGENATED									
Vinylidene chloride and/or dichloroethylene isomer	+[d]	+	+	+	+	+	+	+	+
Methylene chloride	+	+	+	+	+	+	+	+	+
Chloroform	+	+	+	+	+	+	+	+	+
1,2-Dichloroethane	-	-	-	-	T	-	-	-	-
1,1,1-Trichloroethane	-	-	-	+	+	-	-	+	+
Carbon tetrachloride	-	-	+	T	+	+	-	T	+
Trichloroethylene	-	-	-	-	+	-	-	+	+
Tetrachloroethylene	-	-	+	+	+	+	-	+	+
Dichlorobenzene	-	-	T	+	+	-	-	+	+
ALDEHYDES									
Acetaldehyde	+	+	+	+	+	+	+	+	+
Propanal	-	+	-	-	-	-	-	-	-
n-Butanal	-	+	+	+	-	+	-	-	-

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1				Trip 2		Trip 3		
	P1/L4[a]	P2/L5[a]	P3/L2[b]	P3/L6[c]	P2/L3[b]	P3/L5[b]	P1/L9[a]	P2/L8[b]	P2/L9[b]
ALDEHYDES (continued)									
n-Pentanal	-	+	T	+	+	-	-	+	-
n-Hexanal	-	+	+	+	-	T	-	+	-
n-Heptanal	-	-	+	+	-	-	-	+	-
Benzaldehyde	-	-	+	+	+	+	-	+	+
n-Octanal	-	-	+	+	-	+	-	T	+
n-Nonanal	-	-	+	+	+	+	-	+	+
n-Decanal	-	-	+	+	-	+	-	+	+
n-Undecanal	-	-	+	+	-	+	-	+	-
KETONES									
Acetone	+	+	+	+	+	+	+	+	+
Methyl isopropyl ketone	-	-	-	-	-	T	-	-	-
Methyl vinyl ketone	-	-	-	+	-	-	-	-	-
Methyl ethyl ketone	-	-	-	+	+	-	-	T	-
Acetophenone	-	-	+	+	+	+	-	+	+
Benzophenone	-	-	-	+	-	+	-	-	-

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1				Trip 2		Trip 3		
	P1/L4[a]	P2/L5[a]	P3/L2[b]	P3/L6[c]	P2/L3[b]	P3/L5[b]	P1/L9[a]	P2/L8[b]	P2/L9[b]
ESTERS									
Ethyl acetate	-	-	+	-	+	+	-	T	-
ALCOHOLS									
Phenol	-	-	+	+	+	+	-	+	-
Cresol	-	-	+	+	+	+	-	+	-
Dimethylphenol isomer	-	-	+	+	+	+	-	-	-
C_2-alkyl phenol	-	-	+	+	+	+	-	+	-
C_3-alkyl phenol	-	-	+	+	+	+	-	+	-
C_6-alkyl phenol	-	-	+	+	+	-	-	-	-
ETHERS									
Diethyl ether	+	+	+	-	T	T	T	+	+
AROMATICS									
Benzene	+	+	+	+	+	+	-	+	+
Toluene	+	+	+	+	+	+	-	+	+
Ethylbenzene	-	-	+	+	+	+	-	+	+
Styrene	-	-	+	+	+	+	-	+	+
Xylene	-	-	+	+	+	+	-	+	+

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1				Trip 2		Trip 3		
	P1/L4[a]	P2/L5[a]	P3/L2[b]	P3/L6[c]	P2/L3[b]	P3/L5[b]	P1/L9[a]	P2/L8[b]	P2/L9[b]
i- or n-Propylbenzene	-	-	+	+	+	-	-	+	+
Ethyltoluene	-	-	+	+	+	+	-	+	+
Trimethylbenzene	-	-	+	+	+	+	-	+	+
o-Ethyltoluene	-	-	+	-	+	-	-	+	+
C_3-alkyl benzene	-	-	-	-	-	+	-	-	+
C_4-alkyl benzene	-	-	+	+	+	+	-	+	+
Indan	-	-	+	+	+	-	-	+	+
Tetramethylbenzene isomer	-	-	-	-	-	-	-	-	+
C_5-alkyl benzene	-	-	+	+	+	-	-	+	+
C_4H_7 benzene isomer	-	-	-	+	+	-	-	-	-
Naphthalene	-	-	+	+	+	T	-	+	+
C_6-alkyl benzene	-	-	-	-	-	-	-	-	T
β-Methyl naphthalene	-	-	+	+	+	+	-	+	+
α-Methyl naphthalene	-	-	-	+	+	+	-	+	+
C_2-alkyl naphthalene	-	-	-	T	+	-	-	-	-
Biphenyl	-	-	-	+	T	-	-	-	T

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period Location								
	Trip 1				Trip 2		Trip 3		
	P1/L4[a]	P2/L5[a]	P3/L2[b]	P3/L6[c]	P2/L3[b]	P3/L5[b]	P1/L9[a]	P2/L8[b]	P2/L9[b]
SULFUR CONTAINING									
SO_2	-	-	-	-	-	-	-	-	+
CS_2	+	+	-	+	+	-	+	-	+

Notes
- a) Carbon cartridges interpreted.
- b) Tenax GC cartridge interpreted.
- c) Both Tenax GC and carbon cartridges interpreted.
- d) + = identified
  - = not identified
  T = tentative identification

[alkanes, alkenes, and artifacts not included].

Table 19. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM FRONT ROYAL, VA --- TRIP 1

Chemical	Period/Location								
	P1/L1	P1/L2	P1/L3	P1/L4	P2/L3	P2/L5	P3/L2	P3/L6	B
methylene chloride	1000	T(714)	1857	2143	97627	2444	4600	1000	∿6
chloroform	T(125)	125	125	208	4800	149	278	T(125)	≤3
carbon tetrachloride	<95	<95	T(95)	<95	190	T(74)	T(125)	T(95)	≤2
vinyl chloride	<12000	<12000	<12000	<12000	<11538	<10000	<15000	<12000	<15
1,2-dichloroethylene	T(334)	<334	<334	T(500)	<357	<263	<454	<334	≤10
1,1-dichloroethane	<285	<285	<285	<285	<258	<228	<476	<285	<8
1,2-dichloroethane	<258	<258	<258	<258	<500	<195	T(348)	<258	≤8
1,1,1-trichloroethane	T(334)	T(100)	T(334)	T(334)	381	T(278)	<667	T(334)	<5
1,1,2-trichloroethane	<250	<334	<250	<250	<98	<217	<294	<250	<5
trichloroethylene	<100	<100	<100	T(100)	T(98)	T(74)	T(132)	<100	≤5
tetrachloroethylene	T(36)	20	<36	T(36)	132	26	35	31	<7
1,1,1,2-tetrachloroethane	<22	<30	<30	<30	<30	<22	<40	<30	<6
1,1,2,2-tetrachloroethane	<22	<30	<30	<30	<30	<22	<40	<30	<6
pentachloroethane	<7	<15	<8	<22	<7	<9	<9	<15	<5
hexachloroethane	<7	<15	<8	<22	<7	<9	<9	<15	<5
chlorobenzene	<32	<45	<32	<66	<32	T(26)	T(44)	<46	<15
o-dichlorobenzene	<14	<30	<18	<44	T(13)	T(18)	<18	T(31)	<10
m-dichlorobenzene	<14	T(27)	T(18)	22	8	T(18)	T(17)	T(31)	<10
p-dichlorobenzene	<13	<27	<15	<39	<12	<16	<16	<28	<9
1,2,4-trichlorobenzene	<8	<18	<9	<26	<8	<10	<10	<10	<6
1,3,5-trichlorobenzene	<7	<15	<8	<22	<7	<9	<9	<15	<5
1,2,5-trichlorobenzene	<8	<18	<9	<26	<8	<10	<10	<18	<6
vinylidene chloride	<334	<334	<334	T(500)	2500	<263	778	<334	<10

Values in ng/m^3.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is preceeded by <.

B = blank control. Values are in ng/cartridge.

Table 20. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM FRONT ROYAL, VA --- TRIP 2

Chemical	Period/Location								
	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L1	P2/L2	P2/L3	P2/L5
methylene chloride	8375	40571	11428	120142	87375	25250	2625	111556	238250
chloroform	692	792	T(125)	2708	1807	711	T(115)	2193	14517
carbon tetrachloride	217	T(95)	T(95)	1190	T(87)	T(87)	565	889	280
vinyl chloride	<12000	<12000	<12000	<12000	<11750	<12000	<11750	<10000	<11500
1,2-dichloroethylene	T(312)	T(334)	T(334)	T(334)	T(312)	T(312)	T(312)	1842	2974
1,1-dichloroethane	<267	<285	285	<285	<267	<267	<334	<263	<242
1,2-dichloroethane	T(242)	T(258)	T(258)	322	<242	T(242)	T(242)	<228	<205
1,1,1-trichloroethane	T(294)	800	T(334)	2933	T(294)	T(470)	T(470)	195	T(312)
1,1,2-trichloroethane	<227	<250	<250	<250	<227	<363	<227	2500	<238
trichloroethylene	T(96)	T(100)	T(100)	420	<96	T(96)	T(96)	<218	T(77)
tetrachloroethylene	380	332	36	2994	T(36)	163	35	388	77
1,1,1,2-tetrachloroethane	<15	<30	<30	<33	<30	<16	<27	810	<22
1,1,2,2-tetrachloroethane	<15	<30	<30	<33	<30	<16	<27	<22	<22
pentachloroethane	<12	<12	<11	<27	<11	<13	<8	<22	<6
hexachloroethane	<12	<12	<11	<27	<11	<13	<8	<7	<6
chlorobenzene	T(38)	T(36)	T(32)	T(82)	<33	<39	<32	<7	<18
o-dichlorobenzene	58	T(24)	T(21)	T(55)	<22	<26	<15	38	<12
m-dichlorobenzene	35	T(24)	T(21)	279	<22	T(26)	<15	T(14)	<12
p-dichlorobenzene	<23	<22	<19	<49	<20	<23	<14	68	<10
1,2,4-trichlorobenzene	<15	<14	<13	<33	<13	<16	<9	<13	<7
1,3,5-trichlorobenzene	<12	<12	<11	<27	<11	<13	<8	<9	<6
1,2,5-trichlorobenzene	<15	<14	<13	<33	<13	<16	<9	<7	<7
vinylidene chloride	<312	434	<334	<334	<312	<312	<312	<9	<27

Values in ng/m^3.
T = trace, values in parentheses are detection limits.
Where no compound was detected, the detection limit is listed preceeded by <.

Table 21. ESTIMATED LEVEL OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR FROM FRONT ROYAL, VA --- TRIP 3

Chemical	Period/Location									
	B	P1/L2	P1/L4	P1/L7	P1/L8	P1/L9	P2/L2	P2/L7	P2/L8	P2/L9
methylene chloride	≤5	1364	T(454)	2545	<454	1091	1818	2090	6273	<454
chloroform	≤3	T(71)	<71	<71	<71	<71	<71	T(71)	119	<71
carbon tetrachloride	<2	<59	T(59)	<59	<59	<59	T(59)	<59	T(59)	<59
vinyl chloride	<15	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500
1,2-dichloroethylene	<10	T(213)	T(213)	T(213)	<213	T(213)	T(213)	T(213)	T(213)	T(213)
1,1-dichloroethane	<8	<160	<160	<160	<160	<160	<160	<160	<160	<160
1,2-dichloroethane	≤8	T(151)	<151	T(151)	<151	T(151)	T(151)	T(151)	T(151)	T(151)
1,1,1-trichloroethane	≤5	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)
1,1,2-trichloroethane	<5	<167	<167	<167	<167	<167	<167	<167	<167	<167
trichloroethylene	<5	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)
tetrachloroethylene	<7	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)
1,1,1,2-tetrachloroethane	<6	<16	<16	<16	<16	<16	<16	<16	<16	<16
1,1,2,2-tetrachloroethane	<6	<16	<16	<16	<16	<16	<16	<16	<16	<16
pentachloroethane	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6
hexachloroethane	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6
chlorobenzene	≤15	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)
o-dichlorobenzene	<10	T(9)	<9	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)
m-dichlorobenzene	<10	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)
p-dichlorobenzene	<9	<7	<7	<7	<7	<7	<7	<7	<7	<7
1,2,4-trichlorobenzene	<6	<7	<7	T(7)	<7	<7	<7	<7	<7	<7
1,3,5-trichlorobenzene	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6
1,2,3-trichlorobenzene	<6	<7	<7	<7	<7	<7	<7	<7	<7	<7
vinylidene chloride	<10	<213	<213	<213	<213	<213	<213	<213	<213	<213

Values in ng/m^3.
T = trace, values in parentheses are detection limits.
Where no compound was detected, the detection limit is listed preceeded by <.
B = blank control. Values are in ng/cartridge.

Table 22. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM FRONT ROYAL, VA[a] --- TRIP 1

Chemical	Period/Location									
	B	P1/L1	P1/L2	P1/L3	P1/L4	P2/L3	P2/L5	P3/L2	P3/L3	P3/L6
benzene	≤3	722	231	161	52	2481	1167	426	3526	142
toluene	≤3	171	265	151	96	3290	1066	302	4659	280
naphthalene	≤3	18	26	13	<13	196	210	26	196	71
acetophenone	≤10	<14	256	94	123	654	329	127	655	283
n-octanal	≤10	49	47	T(22)	<44	69	T(22)	31	77	37
benzophenone	≤10	32	40	T(15)	<44	17	83	55	<17	52
phenol	≤15	45	80	15	30	137	114	44	137	77
diphenyl ether	<10	14	30	T(15)	<44	16	<44	<22	T(17)	T(31)
ethyl acetate	<7	T(97)	T(21)	T(146)	<65	194	<97	T(97)	292	<65
cyanobenzene	<5	<10	<15	<8	<22	<9	<22	<11	<9	<15
dimethyldisulfide	<8	<163	<235	<238	<113	<14	<35	<163	<235	<25

Values in ng/m^3.
T = trace, values in parentheses are detection limits
Where no compound was detected, the detection limit is listed preceeded by <.
B = blank control. Values are in ng/cartridge.

Table 23. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM FRONT ROYAL, VA[a] ---TRIP 2

	Period/Location									
Chemical	B	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L1	P2/L2	P2/L3	P2/L5
benzene	<3	6334	574	9500	24389	55	685	611	10111	2667
toluene	<3	3957	400	8547	3918	45	461	387	10384	2767
naphthalene	<3	416	27	367	634	T(7)	34	24	442	154
acetophenone	<10	209	70	240	3721	T(22)	27	48	761	327
n-octanal	<10	30	24	132	524	T(22)	50	T(22)	157	107
benzophenone	<10	<25	24	<63	<164	T(22)	T(26)	T(15)	50	179
phenol	<15	128	34	462	967	T(33)	T(39)	12	225	77
diphenyl ether	<10	T(25)	24	<63	<164	T(22)	<26	<15	<14	35
ethyl acetate	<7	118	T(97)	667	583	<97	T(97)	T(97)	361	500
cyanobenzene	<5	<36	12	10	<82	<11	<13	<10	<30	<30
dimethyldisulfide	<8	T(489)	<163	<490	< 490	<163	T(163)	<163	<489	<489

Values in ng/m^3.
T = trace, values in parentheses are detection limits.
Where no compound was detected, the detection limit is preceeded by <.
B = blank control. Values are in ng/cartridge.

Table 24. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM FRONT ROYAL, VA[a]---TRIP 3

Chemical	B	P1/L2	P1/L4	P1/L7	P1/L8	P1/L9	P2/L2	P2/L7	P2/L8	P2/L9
		Period/Location								
benzene	≤3	380	583	778	509	592	231	518	361	481
toluene	≤3	140	395	322	269	113	160	61	421	569
naphthalene	≤3	11	42	24	45	8	11	30	33	21
acetophenone	<10	9	76	126	91	146	69	90	71	40
n-octanal	<10	T(18)	T(21)	T(17)	T(18)	T(18)	T(18)	40	<18	18
benzophenone	<10	T(12)	<21	<10	<16	19	18	<9	<18	<8
phenol	<15	12	13	20	T(23)	26	11	7	17	T(12)
diphenyl ether	<10	<14	<21	<10	<11	<14	19	<9	<18	<8
ethyl acetate	<7	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)
cyanobenzene	≤5	22	T(10)	34	13	28	T(9)	22	<9	<8
dimethyldisulfide	<8	<77	<77	<77	<77	<77	<77	<77	<77	T(77)

Values in ng/m^3.
T = trace, values in parentheses are detection limits.
Where no compound was detected, the detection limit is preceeded by <.
B = blank control. Values are in ng/cartridge.

night-time effects discussed above may have been applicable to this sample. The volatile organic levels during Trip 3 were generally low.

The most striking feature of the halogenated organic quantitation is the high levels of the C_1 halocarbons (methylene chloride, chloroform and carbon tetrachloride). Levels of 1,2-dichlorethylene were significant in two samples (Trip 2, P2/L3 and P2/L5) which were collected overnight. Levels of vinylidene chloride were significant in two samples collected during Trip 1 (P2/L3 and P3/L2).

Semivolatiles

The compounds identified in the toluene and methanol extracts of the <1.7 μ fraction of air particulate from Front Royal are presented in Appendix F. The corresponding peaks are shown in the total ion current (TIC) chromatograms in Appendix F. The computer scales the TIC chromatograms to the most intense peak, so quantitative comparison of the two fractions is not possible.

DISCUSSION

Many more compounds were identified with greater frequency in the Kanawha Valley than in the Shenandoah Valley. This is especially noticeable in the pollutants potentially arising from industrial activity (halogenated and oxygenated compounds). Many compounds, including the aromatics, result from combustion (e.g. automobile exhaust) or other sources which could be considered ubiquitous. This qualitative comparison is in keeping with the greater industrial diversity and higher population density of the Kanawha Valley.

In contrast to the qualitative data, the quantitative data showed much higher levels of most organic pollutants in the Shenandoah Valley than in the Kanawha Valley. This is especially noteworthy, since the Shenandoah Valley is broader and less well-defined and is therefore not expected to be as good an emission reservoir as the Kanawha Valley. The high levels in the Shenandoah Valley were found on both Trips 1 and 2, implying that the levels found are not fortuitous.

The origins of the high levels of pollutants in the Shenandoah and Kanawha Valleys are not discernible from these data, since wind directions were inconsistent during most of the sampling.

It appears from the results presented here that the highest concentrations of pollutants in the Shenandoah Valley occur at night. Therefore, future sampling efforts should make more direct comparisons between day and night levels at the same locations.

SECTION 8

QUALITY CONTROL

Quality control was recognized as an integral and primary component of this program. As such, a rigorous quality assurance program was established to prevent contamination or loss of sample, mislabeling, and to provide estimates on the accuracy of the data. The essential features of the quality control program are discussed below.

SAMPLING

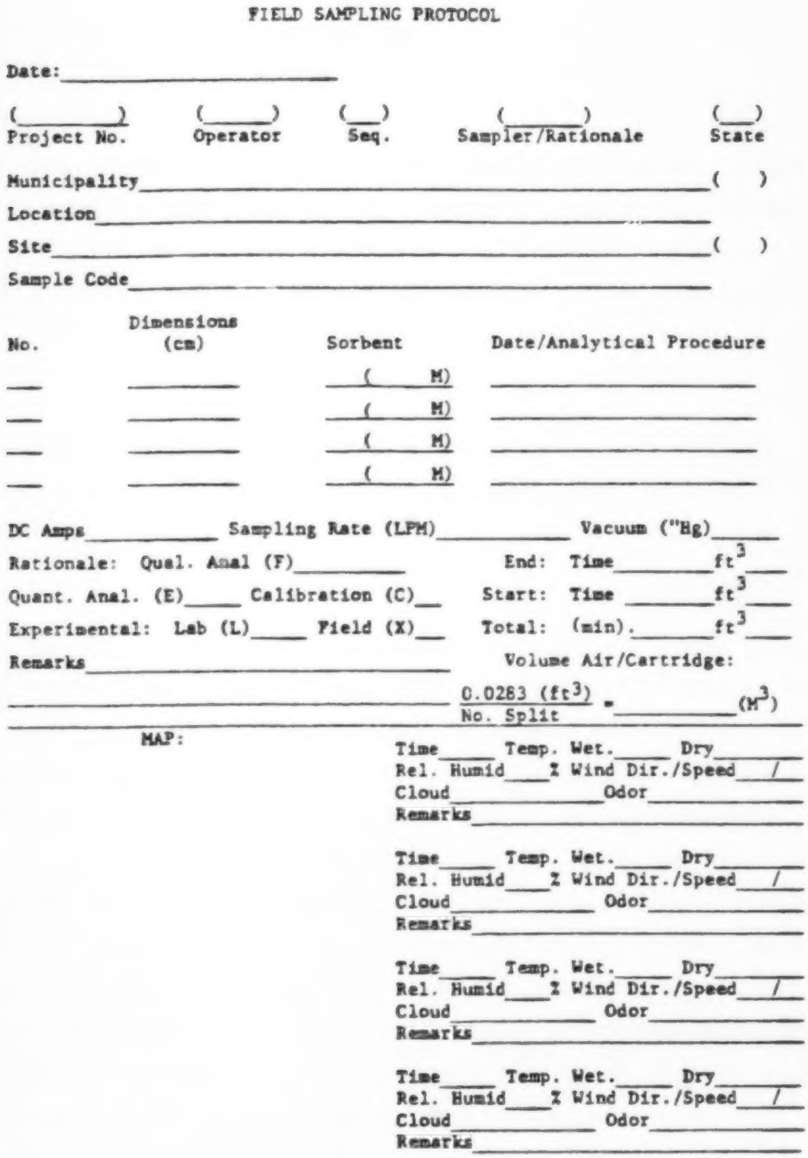
The quality control program used for the sampling of ambient air included sample and data logging, reagent and glassware control, and control samples as discussed below.

Sample Collection

During sample collection, a sample data sheet (Figure 11) was maintained for each sample. The sampling locations for each sampling period were recorded on a detailed area map. The coded form contained information such as date and time of sampling, locations, sampling parameters and meteorological information. The alpha-numeric sample code was also fixed directly to the sample container at that time.

Following each day's sample collection, the protocol sheets and sample labels were independently reviewed by two field personnel to assure that all information was logged in, that the codes were self-consistent and that there was no duplication. Upon returning to the laboratory, the samples were again checked for proper labeling. Upon submission for analysis, the samples were logged in by the GC/MS/COMP operator and a running account of sample analysis and data output maintained. When the sample analysis and data output were completed, the data were returned to the Project Director and logged in.

Each sample was collected on duplicate cartridges in parallel. Thus, additional quality assurance was provided not only in case of sample damage, but also for confirmatory analysis if necessary.



FIELD SAMPLING PROTOCOL

Date:________________________

(________) (______) (__) (_______) (__)
Project No. Operator Seq. Sampler/Rationale State

Municipality____( )

Location____

Site____( )

Sample Code____

No.	Dimensions (cm)	Sorbent	Date/Analytical Procedure
___	__________	(M)	______________________
___	__________	(M)	______________________
___	__________	(M)	______________________
___	__________	(M)	______________________

DC Amps__________ Sampling Rate (LPM)__________ Vacuum ("Hg)______

Rationale: Qual. Anal (F)__________ End: Time________ft^3___

Quant. Anal. (E)_____ Calibration (C)__ Start: Time ________ft^3___

Experimental: Lab (L)_____ Field (X)__ Total: (min).________ft^3___

Remarks______________________________ Volume Air/Cartridge:

______________________________ $\frac{0.0283\ (ft^3)}{\text{No. Split}}$ = __________(M^3)

MAP:

Time_____ Temp. Wet._____ Dry_______
Rel. Humid___% Wind Dir./Speed___/___
Cloud____________Odor____________
Remarks____________________

Time_____ Temp. Wet._____ Dry_______
Rel. Humid___% Wind Dir./Speed___/___
Cloud____________ Odor____________
Remarks____________________

Time_____ Temp. Wet._____ Dry_______
Rel. Humid___% Wind Dir./Speed___/___
Cloud____________ Odor____________
Remarks____________________

Time_____ Temp. Wet._____ Dry_______
Rel. Humid___% Wind Dir./Speed___/___
Cloud____________ Odor____________
Remarks____________________

Figure 11. Field Sampling Protocol Data Sheet.

Reagent and Glassware Control

Reagent and glassware control was required in order to minimize contamination. Sample containers, glassware, etc. were cleaned with Isoclean®, rinsed with deionized-distilled water and heat treated at 450-500°C to insure the removal of all traces of organic compounds. Solvents were redistilled in glass in our laboratories prior to their use.

Quality Control Samples

Blank sampling cartridges and control cartridges loaded with known amounts of standards were prepared for each sampling trip. Half of the samples were designated "lab blanks/controls" and remained in the laboratory, the other half were designated "field blanks/controls", and were carried to the field in the same containers as the sampling cartridges. The quality control scheme is outlined in Table 25 . This procedure not only provided a check of possible contamination during transportation and storage, but also allowed calculation of overall recoveries during the storage and analysis phases.

SAMPLE WORKUP AND ANALYSIS

Volatiles Collected on Tenax GC Cartridges

The quality assurance program consisted of analysis of controls and blanks, cross-checking data interpretation, and validation of methodology.

The results of the blank analyses are included with the quantitation results (Tables 15, 16, 19, 21-24). The recoveries of selected organic compounds from Tenax GC cartridges are listed in Table 10. The results from Trip 3 are not included because the standards were improperly loaded onto the cartridges. The recoveries shown are very good, considering that each cartridge was stored at ambient temperature for up to one week during sampling. These results indicate that sample loss from the cartridges during storage is minimal.

The qualitative data presented in Appendices C-F were independently checked after interpretation.

The entire method has been previously validated.(1-7,11,12)

Highly Volatile Compounds Collected on Carbon Cartridges

The quality control program for these samples was essentially the same as for the samples collected on Tenax GC. The recoveries of compounds on

Table 25. CONTROL SAMPLES FOR EACH FIELD SAMPLING TRIP.

Sample Type	Blank[a] (Lab)	Blank[b] (Field)	Controls[a] (Lab)	Controls[b] (Field)	Total
Tenax Cartridges	2	2	2[c]	2[c]	8
Carbon Cartridges	2	2	2[d]	2[d]	8

---

[a] Remain in laboratory, stored with samples on return.

[b] Travel with samples to the field and return.

[c] Cartridges were loaded with benzene (240.5 ng), methylene chloride (300 ng), toluene (110 ng), 1,1,1-trichloroethane (35 ng), chloroform (200 ng) and methyl ethyl ketone (194 ng).

[d] Cartridges were loaded with methyl chloride (310 ng) and methyl bromide (100 ng).

the controls were not quantitated since no compounds of interest were found in the field samples. The method has been thoroughly validated on previous contracts.(7,11,12)

Particulate Collected on MAS

Since there was no suitable method of preparation of control and blank samples and quantitation was not attempted, no quality control samples were used.

As discussed above, the extraction method was validated for a broad range of organic compounds.

The data interpretation is described above. It was necessary to employ two independent interpretors to assure that identifications were correct. This procedure was especially critical for the semi-volatiles (vis á vis the compounds collected on Tenax GC) due to the large number of possible compounds present, and the relative state of the art.

Summary

In summary, measures were taken to assure that both the qualitative and quantitative data generated under this study are accurate and complete.

REFERENCES

1. Pellizzari, E. D., Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. Publication No. EPA-600/2-75-076, Contract No. 68-02-1228, 185 pp., November, 1975.
2. Pellizzari, E. D., The Measurement of Carcinogenic Vapors in Ambient Atmospheres, Publication No. EPA-600/7-77-055, Contract No. 68-02-1228, 288 pp., June, 1977.
3. Bursey, J. T., D. Smith, J. E. Bunch, R. N. Williams, R. E. Berkley, and E. D. Pellizzari, Amer. Lab., December, 1977, 35-41.
4. Pellizzari, E. D., J. E. Bunch, R. E. Berkley and J. McRae, Anal. Lett., 9, 45 (1976).
5. Pellizzari, E. D., Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy, Publication No. EPA-600/2-77-100, Contract No. 68-02-2262, 104 pp., June, 1977.
6. Zweidinger, R. A., Analysis of Organic Emissions of Automobile Interiors and Quantitation of Vinyl Chloride Monomer, Interim Report, EPA Contract No. 68-02-1325, Task 63, in preparation.
7. Pellizzari, E. D., Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. Publication No. EPA-650/2-74-121, Contract No. 68-02-1228, 148 pp., July, 1974.
8. Mitchell, R. I., W. M. Henry, N. C. Henderson, R. J. Thompson and R. M. Burton, N. C. Henderson, "Massive Volume Sampler for Gram Quantities of Respirable Aerosols (Mark II)". Presented at Meeting of the Air Pollution Control Association, June 22-24, 1977, Toronto, Ont.
9. Henry, W. M. and R. I. Mitchell, "Collection and Analysis of Airborne Suspended Particulate Matter Respirable to Humans for Sulfonates and Polycyclic Organics", Final Report, EPA Contract No. 68-02-0752, May, 1975.
10. Pellizzari, E. D., The Measurement of Carcinogenic Vapors in Ambient Atmospheres, EPA-600/7-77-055, June, 1977.

11. Pellizzari, E. D., Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy, EPA-600/2-77-100, June, 1977.

12. Virginia State Chamber of Commerce, Industrial Directory of Virginia, 10th ed., Richmond, 1969-70.

13. L. W. Little, "Application of *Salmonella typhimurium* Histidine-Deficient Strains to the Screening of Selected Air Pollutants for Potential Carcinogenicity," EPA Contract No. 68-02-2724, Quarterly Technical Progress Report No. 2, January, 1978.

APPENDIX A

SAMPLING AND ANALYSIS FOR VOLATILE ORGANICS IN AMBIENT AIR

APPENDIX A

SAMPLING AND ANALYSIS FOR VOLATILE ORGANICS IN AMBIENT AIR

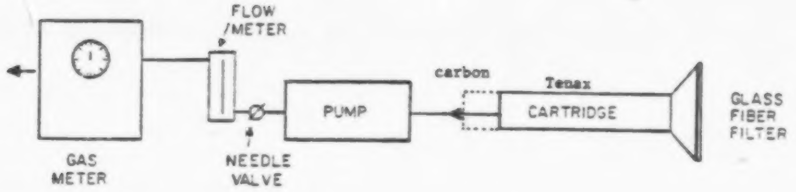
1.0 Principle of Method

Volatile organic compounds are concentrated from ambient air on Tenax GC in a short glass tube (1-3). Recovery of the volatile organics is accomplished by thermal desorption and purging with helium into a liquid nitrogen cooled nickel capillary trap (1,2,4) and the vapors then introduced onto a high resolution glass gas chromatographic column where the constituents are separated from each other (2,5). Characterization and quantitation of the constituents in the sample are accomplished by mass spectrometry, either by measuring the intensity of the total ion current signal or mass fragmentography (2,6). The collection and analysis systems are shown in Figure A-1.

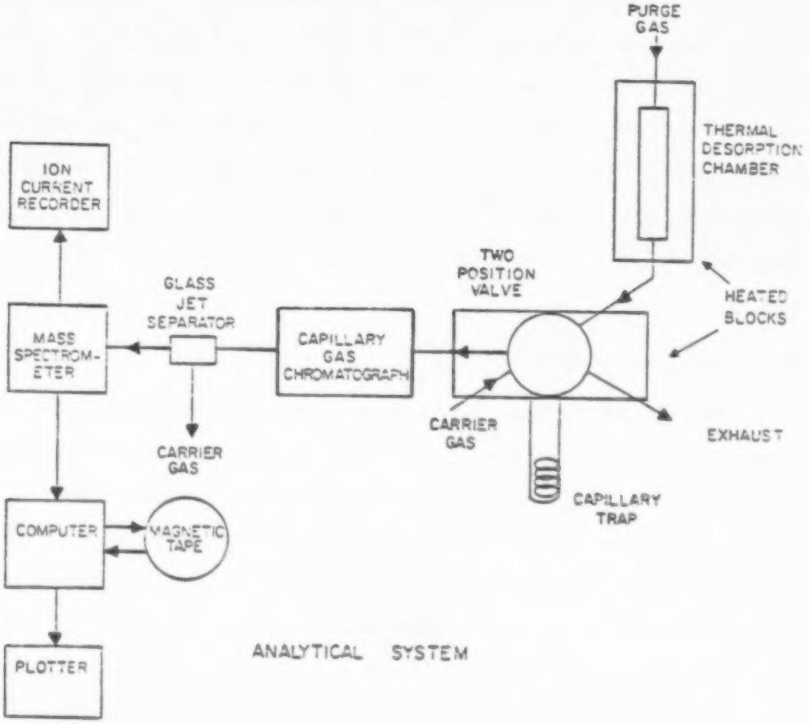
2.0 Range and Sensitivity

The linear range for the analysis of volatile organic compounds depends upon two principal features. The first is a function of the breakthrough volume of each specific compound trapped on the Tenax GC sampling cartridge, and the second is related to the inherent sensitivity of the mass spectrometer for each organic compound (2,7). Thus, the range and sensitivity is a direct function of each compound which is present in the original ambient air. The linear range for quantitation on the gas chromatograph/mass spectrometer/computer (GC/MS/COMP) is generally three orders of magnitude. Table A-1 lists the overall theoretical sensitivity for some examples of volatile organics which is based on these two principles (7).

The sensitivity of this technique for the very volatile compounds (C_1 to C_5) is inadequate for the purpose of this study. Alternate methods for their collection and analysis are suggested.


FLOW
/METER
carbon
Tenax
PUMP
CARTRIDGE
GLASS
FIBER
FILTER
GAS
METER
NEEDLE
VALVE

VAPOR COLLECTION SYSTEM


PURGE
GAS
THERMAL
DESORPTION
CHAMBER
ION
CURRENT
RECORDER
TWO
POSITION
VALVE
GLASS
JET
SEPARATOR
HEATED
BLOCKS
MASS
SPECTROM-
ETER
CAPILLARY
GAS
CHROMATOGRAPH
CARRIER
GAS
EXHAUST
CARRIER
GAS
CAPILLARY
TRAP
COMPUTER
MAGNETIC
TAPE
PLOTTER

ANALYTICAL SYSTEM

Figure A-1. Vapor collection and analytical systems for analysis of organic vapors in ambient air.

Table A-1. OVERALL THEORETICAL SENSITIVITY OF HIGH RESOLUTION GAS CHROMATOGRAPHY/MASS SPECTROMETRY/COMPUTER ANALYSIS FOR ATMOSPHERIC POLLUTANTS

Chemical Class		Estimated Detection Limit[a]	
		ng/m^3	ppt
Halogenated hydrocarbon	Vinyl bromide	250	57
	Bromoform	0.340	0.03
	Bromodichloromethane	1.300	0.22
	Dibromochloromethane	0.667	0.07
	1-Bromo-2-chloroethane	1.00	0.67
	Allyl bromide	5.00	1.04
	1-Bromopropane	5.200	1.06
	1-Chloro-3-bromopropane	0.150	0.01
	1-Chloro-2,3-dibromopropane	~0.100	<0.01
	1,1-Dibromo-2-chloropropane	~0.100	<0.01
	1,2-Dibromoethane	0.530	0.07
	1,3-Dibromopropane	~0.100	~0.01
	Epichlorohydrin (1-Chloro-2,3-epoxypropane)	9.600	2.50
	Epibromohydrin (1-Bromo-2,3-epoxypropane)	0.300	0.05
	Bromobenzene	0.100	0.02
	Methyl bromide	500	135
	Methyl chloride	2000	1000
	Vinyl chloride	800	333
	Methylene chloride	700	200
	Chloroform	200	420
	Carbon tetrachloride	250	400

(continued)

Table A-1 (continued)

Chemical Class	Compound	Estimated Detection Limit[a]	
		ng/m^3	ppt
Halogenated hydrocarbon (cont'd)	1,2-Dichloroethane	32	8.15
	1,1,1-Trichloroethane	66	12.45
	Tetrachloroethylene	2.5	0.38
	Trichloroethylene	10	1.92
	1-Chloro-2-methylpropene	62	21.5
	3-Chloro-2-methylpropene	62	21.5
	3-Chloro-1-butene	83	28.8
	Allyl chloride	83	28.8
	4-Chloro-1-butene	38	13.2
	1-Chloro-2-butene	13	4.5
	Chlorobenzene	2.10	0.47
	o-Dichlorobenzene	1.00	0.06
	m-Dichlorobenzene	0.75	0.01
	Benzylchloride	0.65	0.01
Halogenated ethers	2-Chloroethyl ethyl ether	4.15	0.97
	Bis-(chloromethyl)ether	1.0	1.10
Nitrosamines	N-Nitrosodimethylamine	5.0	1.67
	N-Nitrosodiethylamine	3.0	0.74
Oxygenated	Acrolein	~100	56.5
	Glycidaldehyde	~59	19.5
	Propylene oxide	~60	25.5
	Butadiene diepoxide	~20	6.7

(continued)

Table A-1 (continued)

Chemical Class	Compound	Estimated Detection Limit[a]	
		ng/m^3	ppt
Oxygenated hydrocarbons (continued)	Cyclohexene oxide	~10	2.5
	Styrene oxide	2	0.415
	Acetophenone	~2	~0.415
	β-Propiolactone	~3	~1.2
Nitrogenous Compounds	Nitromethane	8	~2.4
	Aniline	3.0	0.78
Sulfur Compounds	Diethyl sulfate	~50	-
	Ethyl methane sulfate	~5.0	-

[a] Limits are calculated on the basis of the breakthrough volume for 2.2 g of Tenax GC, capillary column performance and sensitivity of the mass spectrometer to that compound in the mass fragmentography mode of most intense ion.

3.0 Interferences

The potential difficulties with this technique are primarily associated with those cases where isomeric forms of a particular substance cannot be resolved by the high resolution chromatographic column and the mass cracking pattern of each of the isomers is identical. An example of such a problem is seen with the C_5-alkyl aromatics of which there are 53 isomers. As the number of carbon atoms increase in the hydrocarbons and aromatics, the number of potential isomers become increasingly large and difficult to completely resolve by gas chromatography and/or by their corresponding mass cracking patterns. However, differentiation between the hydrocarbons, that is alkanes, alkenes, aromatics, oxygenated, etc. can be made. Known background compounds include phthalate esters; silanes, phosphines and thiophosphines (from the SCOT column); 2,2,4-trimethylpenta-1,3-diol-diisobutyrate ("SNOOP"); fluorocarbon refrigerants; and acetic acid (Tenax GC decomposition product).

Interferences in quantitation can usually be avoided by properly setting the computer S/N threshold.

4.0 Reproducibility

The reproducibility of this method has been determined to range from ±10 to ±30 percent of the relative standard deviation for different substances when replicate sampling cartridges are examined (5). The inherent analytical errors are a function of several factors: (1) the ability to accurately determine the breakthrough volume for each of the identified organic compounds, (2) the accurate measurement of the ambient air volume sampled, (3) the percent recovery of the organic from the sampling cartridge after a period of storage, (4) the reproducibility of thermal desorption for a compound from the cartridge and its introduction into the analytical system, (5) the accuracy of determining the relative molar response ratios between the identified substance and the external standard used for calibrating the analytical system, (6) the reproducibility of transmitting the sample through the high resolution gas chromatographic column, and (7) the day-to-day reliability of the ms-comp system (1-8).

The accuracy of the analysis is generally ±30%, however, the accuracy is dependent on the chemical and physical nature of the compound (2,8).

5.0 Advantages and Disadvantages of the Method

The gas chromatograph/mass spectrometer, interfaced with a glass jet separator is extremely sensitive and specific for the analysis of many organic compounds in ambient air. High resolution gas chromatographic separation provides adequate resolution of the substances found in ambient air for their subsequent quantification. The combination of high resolution gas chromatographic column and the selection of specific or unique ions representing the various compounds identified in air samples yields a relatively specific assay method for these compounds (1-8).

Collected samples can be stored up to one month with less than 10% losses for most of the chemical classes (2,8). Because some of the compounds of interest may be hazardous to man, it is extremely important to exercise safety precautions in the preparation and disposal of liquid and gas standards, cleaning of used glassware, etc. and the analysis of air samples.

Since the mass spectrometer cannot be conveniently mobilized, sampling must be carried out away from the instrument.

The efficiency of air sampling increases as the temperature of ambient air decreases (i.e., sensitivity increases) (8).

The retention of water by Tenax is low, its thermal stability is high and its background is negligible allowing sensitive analysis (1,2,5,8).

6.0 Apparatus

6.1 Sampling Cartridges

The sampling tubes are prepared by packing a 10 cm long x 1.5 cm i.d. glass tube with 6.0 cm of 35/60 mesh Tenax GC, placing glass wool in the ends to provide support (2,5). Virgin Tenax (or material to be recycled) is extracted in a Soxhlet extractor for a minimum of 48 hours with methanol and pentane prior to preparation of cartridge samplers (2,5). After purification of the Tenax GC sorbent and drying in a vacuum oven at 100°C for 16 hr at a vacuum of 28 inches of water, all the sorbent material is meshed to provide a 35/60 particle size range. Cartridge samplers are then prepared and conditioned at 270°C with helium flow at 30 ml/min for 30 minutes. The conditioned cartridges are transferred to Kimax® (2.5 cm x 150 cm) culture tubes, immediately sealed using Teflon lined caps, and cooled. This procedure is performed in order to avoid recontamination of the sorbent bed (2,5).

Cartridge samplers with longer beds of sorbent may be prepared using a proportional increase in the amount of Tenax GC in order to achieve a larger breakthrough volume for each compound and thus increasing the overall sensitivity of the technique (8).

6.2 Gas Chromatographic Column

A 0.35 mm i.d. x 100 m glass SCOT capillary column coated with SE-30 stationary phase and 0.1% benzyltriphenylphosphonium chloride is used for effecting the resolution of the volatile organic compounds (5). The capillary column is conditioned for 48 hr at 245°C at a 2.25 ml/min helium flow.

A glass jet separator on a Varian-MAT CH-7 GC/MS/COMP system is employed to interface the glass capillary column to the mass spectrometer. The glass jet separator is maintained at 240°C (2.5).

6.3 Inlet Manifold

An inlet manifold for thermally recovering vapors trapped on Tenax sampling cartridges is employed and is shown in Figure A-1 (1,2,4,5).

6.4 Gas Chromatograph

A Varian 1700 gas chromatograph is used to house the glass capillary column and is interfaced to the inlet manifold (Fig A-1).

6.5 Mass Spectrometry/Computer

A Varian-MAT CH-7 mass spectrometer with a resolution of 2,000 equipped with a single ion monitoring capability is used in tandem with the gas chromatograph (Fig. A-1). The mass spectrometer is interfaced to a Varian 620/L computer (Fig. A-1).

7.0 Reagents and Materials

All reagents used are analytical reagent grade.

8.0 Procedure

8.1 Cleaning of Glassware

All glassware, sampling tubes, cartridge holders, etc. are washed in Isoclean®/water, rinsed with deionized distilled water, acetone and air dried. Glassware is heated to 450-500°C for 2 hours to insure that all organic material has been removed prior to its use.

8.2 Collection of Halogenated Hydrocarbons in Ambient Air

Continuous sampling of ambient air is accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Fig. A-1, ref. 2). Flow rates are maintained at 1-10 ℓ/min are available with the system. Flow rates are generally maintained at 1 ℓ/min using critical orifices, and the total flow is monitored through a calibrated flow meter. The total flow is also registered by a dry gas meter. Concomitant with these parameters the temperature is continuously recorded with a Meteorology Research Incorp. Weather Station since the breakthrough volume is important in order to obtain quantitative data on the volatile organics. This portable sampling unit operates on a 12 volt storage battery and is capable of continuous operation up to a period of 24 hours. However, in most cases, the sampling period will consist of 1 to 3 hours at the rates which will be employed in the field. This portable sampling unit will be utilized for obtaining "high volume" samples. Duplicate cartridges are deployed on each sampling unit utilizing a sampling head as shown in Figure A-2.

In addition to the Nutech samplers five duPont personnel samplers are used to sample "low volumes" of ambient air as well as long term integrated samples (12-36 hr). Identical Tenax GC sampling cartridge are employed in this case, and sampling is conducted in duplicate. The flow rate is balanced between duplicate cartridges using critical orifices to maintain a rate of 25 or 100 ml/min/cartridge.

For large sample volumes it is important to realize that a large volume of air may cause elution of compounds through the sampling tube if their breakthrough volume is exceeded. The breakthrough volumes of some volatile organics are shown in Table A-2 (2,4,7,8). These breakthrough volumes have been determined by a previously described technique (2). The breakthrough volume is defined as that point at which 50% of a discreet sample introduced into the cartridge is lost. Although the identity of a compound during ambient air sampling is not known (therefore also its breakthrough volume) the compound can still be quantified, after identification by GC/MS/COMP, once the breakthrough volume been been established. Thus the last portion of the sampling period corresponding to the breakthrough volume is selected for calculating their concentration.

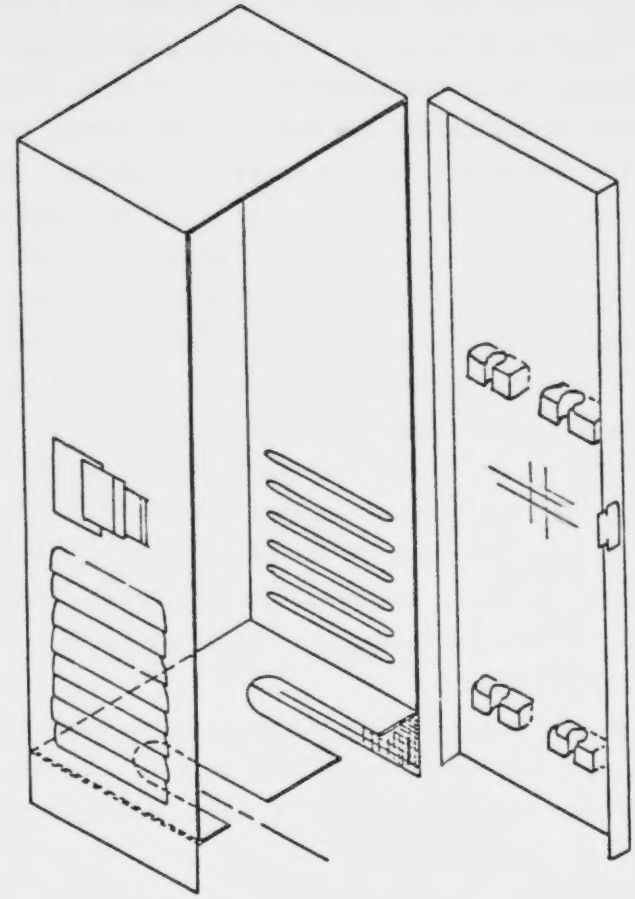


Figure A-2. Sampling head for housing cartridge sampling train.

Table A-2. BREAKTHROUGH VOLUMES FOR SEVERAL ATMOSPHERIC POLLUTANTS[1]

Chemical Class	Compound	b.p. (°C)	Temperature (°F)					
			50	60	70	80	90	100
halogenated hydrocarbon	methyl chloride	-24	0.8	0.6	0.5	0.4	0.3	0.25
	methyl bromide	3.5	3	2	2	1	1	0.9
	vinyl chloride	13	2	1.5	1.25	1.0	0.8	0.6
	methylene chloride	41	11	9	7	5	4	3
	chloroform	61	42	31	24	18	13	10
	carbon tetrachloride	77	34	27	21	16	13	10
	1,2-dichloroethane	83	53	41	31	23	18	14
	1,1,1-trichloroethane	75	23	18	15	12	9	7
	tetrachloroethylene	121	361	267	196	144	106	78
	trichloroethylene	87	90	67	50	38	28	21
	1-chloro-2-methylpropene	68	26	20	16	12	9	7
	3-chloro-2-methylpropene	72	29	22	17	13	10	8
	1,2-dichloropropane	95	229	162	115	81	58	41
	1,3-dichloropropane	121	348	253	184	134	97	70
	epichlorohydrin (1-chloro-2,3-epoxypropane)	116	200	144	104	74	54	39
	3-chloro-1-butene	64	19	15	12	9	7	6
	allyl chloride	45	21	16	12	9	6	5
	4-chloro-1-butene	75	47	36	27	20	15	12
	1-chloro-2-butene	84	146	106	77	56	40	29
	chlorobenzene	132	899	653	473	344	249	181
	o-dichlorobenzene	181	1,531	1,153	867	656	494	372
	m-dichlorobenzene	173	2,393	1,758	1,291	948	697	510
	benzyl chloride	179	2,792	2,061	1,520	1,125	830	612
	bromoform	149	507	386	294	224	171	130
	ethylene dibromide	131	348	255	188	138	101	74
	bromobenzene	155	2,144	1,521	1,079	764	542	384

(continued)

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F)					
			50	60	70	80	90	100
halogenated ethers	2-chloroethyl ethyl ether	108	468	336	241	234	124	89
	Bis-(chloromethyl)ether	-	995	674	456	309	209	142
nitrosamines	N-nitrosodimethylamine	151	385	280	204	163	148	107
	N-nitrosodiethylamine	177	2,529	1,836	1,330	966	700	508
Oxygenated hydrocarbons	acrolein	53	19	14	10	8	6	4
	glycidaldehyde	-	364	247	168	114	77	52
	propylene oxide	34	35	24	17	11	8	5
	butadiene diepoxide	-	1,426	1,009	714	506	358	253
	cyclohexene oxide	132	2,339	1,644	1,153	811	570	400
	styrene oxide	194	5,370	3,926	2,870	2,094	1,531	1,119
	phenol	183	2,071	1,490	1,072	769	554	398
	acetophenone	202	3,191	2,382	1,778	1,327	991	740
	β-propiolactone	57	721	514	366	261	186	132
nitrogenous hydrocarbons	nitromethane	101	45	34	25	19	14	11
	aniline	184	3,864	2,831	2,075	1,520	1,114	817
sulfur compounds	diethyl sulfate	208	40	29	21	15	11	8
	ethyl methane sulfate	86	5,093	3,681	2,564	1,914	1,384	998
amines	dimethylamine	7.4	9	6	4	3	2	1
	isobutylamine	69	71	47	34	23	16	11
	t-butylamine	89	6	5	4	3	2	1
	di-(n-butyl)amine	159	9,506	7,096	4,775	3,105	2,168	1,462
	pyridine	115	378	267	189	134	95	67
	aniline	184	8,128	5,559	3,793	2,588	1,766	1,205
ethers	diethyl ether	34.6	29	21	15	11	8	5
	propylene oxide	35	13	9	7	5	4	3

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F) 50	60	70	80	90	100
esters	ethyl acetate	77	162	108	72	48	32	22
	methyl acrylate	80	164	111	75	50	34	23
	methyl methacrylate	100	736	484	318	209	137	90
ketones	acetone	56	25	17	12	8	6	4
	methyl ethyl ketone	80-2	82	57	39	27	19	13
	methyl vinyl ketone	81	84	58	40	28	19	14
	acetophenone	202	5,346	3,855	2,767	2,000	1,439	1,037
aldehydes	acetaldehyde	20	3	2	2	1	0.9	0.7
	benzaldehyde	179	7,586	5,152	3,507	2,382	1,622	1,101
alcohols	methanol	64.7	1	1	0.8	0.6	0.4	0.3
	n-propanol	97.4	27	20	14	10	7	5
	allyl alcohol	97	32	23	16	11	8	6
aromatics	benzene	80.1	108	77	54	38	27	19
	toluene	110.6	494	348	245	173	122	86
	ethylbenzene	136.2	1,393	984	693	487	344	243
	cumene	152.4	3,076	2,163	1,525	1,067	750	527
hydrocarbons	n-hexane	68.7	32	23	17	12	9	6
	n-heptane	98.4	143	104	75	55	39	29
	1-hexene	63.5	28	20	15	11	8	6
	1-heptene	93.6	286	196	135	93	64	44
	2,2-dimethylbutane	49.7	0.5	0.4	0.3	0.2	0.2	0.1
	2,4-dimethylpentane	80.5	435	252	146	84	49	28
	4-methyl-1-pentene	53.8	14	10	8	6	4	3
	cyclohexane	80.7	49	36	26	19	14	10

(continued)

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F) 50	60	70	80	90	100
inorganic gases	nitric oxide	–	0	0	0	0	0	0
	nitrogen dioxide	–	0	0	0	0	0	0
	chlorine	–	0	0	0	0	0	0
	sulfur dioxide	–	0.06	0.05	0.03	0.02	0.02	0.01
	water	100	0.06	0.05	0.04	0.03	0.01	0

---

[1] Breakthrough volume is given in ℓ/2.2 g Tenax GC used in sampling cartridges.

Previous experiments have shown that organic vapors collected on Tenax GC sorbent are stable and can be quantitatively recovered from the cartridge samplers up to four weeks after sampling when they are tightly closed in cartridge holders and placed in a second container that can be sealed, protected from light, and stored at 0°C (1,2).

8.3 Analysis of Sample

The instrumental conditions for the analysis of volatile organics on the sorbent Tenax GC sampling cartridge are shown in Table A-3. The thermal desorption chamber and the six-port valco valve are maintained at 270° and 240°C, respectively. The glass jet separator is maintained at 240°. The mass spectrometer is set to scan the mass range from 25-350. The helium purged gas through the desorption chamber is adjusted to 15-20 ml/min. The nickel capillary trap at the inlet manifold is cooled with liquid nitrogen. In a typical thermal desorption cycle a sampling cartridge is placed in the preheated desorption chamber and helium gas is channeled through the cartridge to purge the vapors into the liquid nitrogen cooled nickel capillary trap [the inertness activity of the trap has been shown in previous studies (5)]. After the desorption has been completed, the six-port valve is rotated and the temperature on the capillary loop is rapidly raised (greater than 10°/min); the carrier gas then introduces the vapors onto the high resolution glc column. The glass capillary column is temperature programmed from ambient to 240°C at 4°C/min and held at the upper limit for a minimum of 10 min. After all of the components have been eluted from the capillary column, the analytical column is then cooled to ambient temperature and the next sample is processed (2).

An example of the analysis of volatile organics in ambient air is shown in Figure A-3 and the background from a blank cartridge in Figure A-4. The high resolution glass capillary column was coated with SE-30 stationary which is capable of resolving a multitude of compounds for subsequent identification by ms-comp techniques; in this case over 120 compounds were identified in this chromatogram.

8.3.1 Operation of the MS-COMP System (Fig. A-5)

Typically, the mass spectrometer is initially set to operate in the repetitive scanning mode. In this mode the magnet is automatically scanned

Table A-3. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC 100 m glass SCOT-OV101	
50 m glass SCOT-Carbowax 20M	20-240°C, 4/C° min
	80-240°C
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	*m/e* 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	~4 x 10^{-6} torr

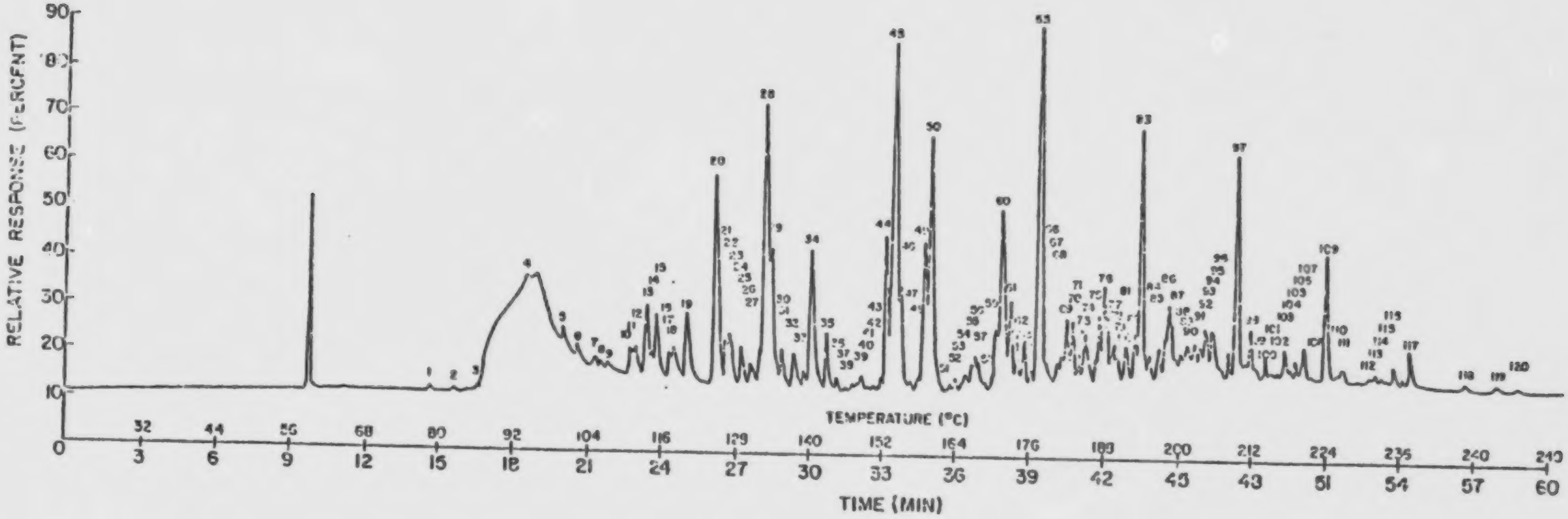


Figure A-3. Profile of ambient air pollutants for Wood River, IL using high resolution gas chromatography/mass spectrometry/computer.

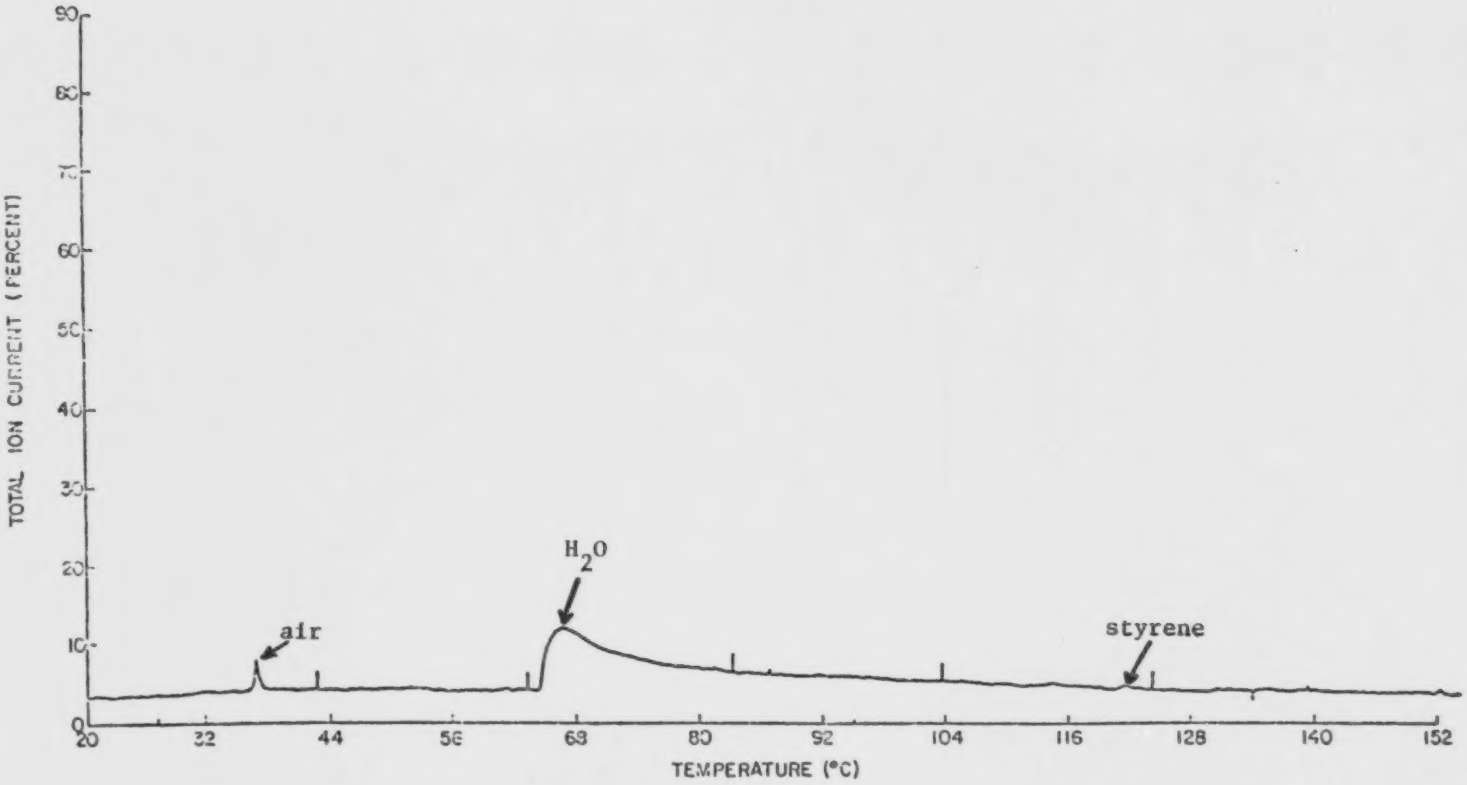


Figure A-4. Background profile for Tenax GC cartridge blank.

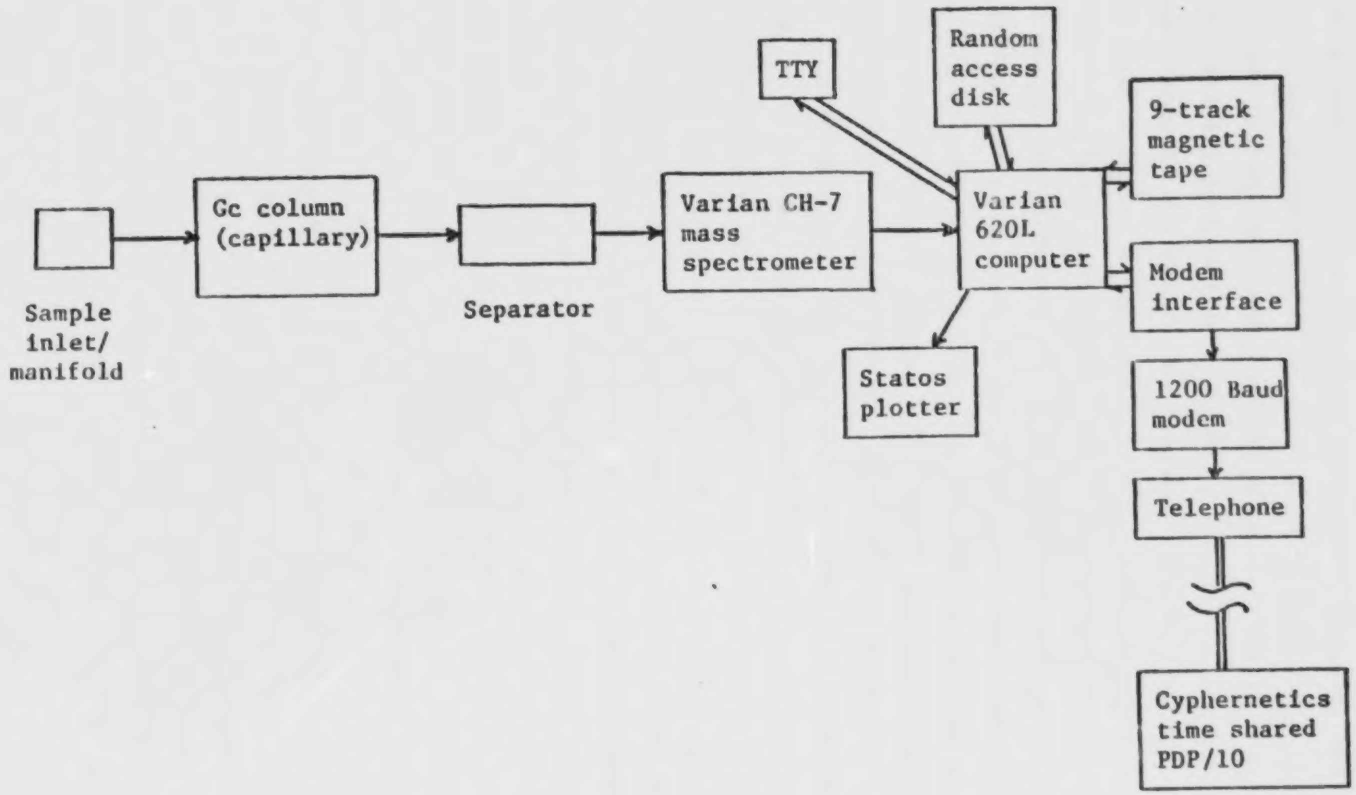

TTY
Random access disk
9-track magnetic tape
Varian 620L computer
Modem interface
Sample inlet/ manifold
Gc column (capillary)
Separator
Varian CH-7 mass spectrometer
Statos plotter
1200 Baud modem
Telephone
Cyphernetics time shared PDP/10

Figure A-5. Schematic diagram of gc-ms computer system exponentially upward from a preset low mass to a high mass value. Although the scan range may be varied depending on the particular sample, the range is typically set from m/e 25 to m/e 300. The scan is completed in approximately 1.8 seconds. At this time the instrument automatically resets itself to the low mass position in preparation for the next scan, and the information is accumulated by an on-line 620/L computer and written onto magnetic tapes or the dual disk system. The reset period requires approximately 20 seconds. Thus, a continuous scan cycle of 3.8 seconds/scan is maintained and repetitively executed throughout the chromatographic run. The results is the accumulation of a continuous series of mass spectra throughout the chromatographic run in sequential fashion.

Prior to running unknown samples the system is calibrated by introducing a standard substance, perfluorokerosene, into the instrument and determining the time of appearance of the known standard peaks in relation to the scanning magnetic field. The calibration curve which is thus generated will be stored in the 620/L computer memory. This calibration serves only to calibrate the mass ion over the mass scanning range.

While the magnet is continuously scanning the sample is injected and automatic data acquisition is initiated. As each spectrum is acquired by the computer, peaks which exceed a preset threshold are recognized and reduced to centroid time and peak intensity. This information is stored in the computer core while the scan is in progress. In addition, approximately 30 total ion current values and an equal number of Hall probe signals are stored in the core of the computer as they are acquired. During the two-second period between scans this spectral information, along with the spectrum number, is written sequentially on disks, and the computer is reset for the acquisition of the next spectrum.

This procedure continues until the entire gc run is completed. By this time there are from 800-1,400 spectra on the disk which are then subsequently processed. Depending on the information required, the data may then either be processed immediately or additional samples may be run, stored on magnetic tape and the results examined at a later time.

The mass spectral data are processed in the following manner. First, the original spectra are scanned and the total ion current (TIC) information is extracted. Then the TIC intensities are plotted against the spectrum number on the Statos 31 recorder. The information will generally indicate whether the run is suitable for further processing, since it will give some idea of the number of unknowns in the sample and the resolution obtained using the particular glc column conditions.

The next stage of the processing involves the mass conversion of the spectral peak times to peak masses which is done directly via the dual disk system. The mass conversion is accomplished by use of the calibration table obtained previously using perfluorokerosene. Normally one set of the calibration data is sufficient for an entire day's data processing since the characteristics of the Hall probe are such that the variation in calibration is less than 0.2 atomic mass units/day. A typical time required for this conversion process for 1,000 spectra is approximately 30 min.

After the spectra are obtained in mass converted form, processing proceeds either manually or by computer. In the manual mode the full set of spectral from the gc run are recorded on the Statos 31 plotter. The TIC information available at this time is most useful for deciding which spectra are to be analyzed. At the beginning of the runs where peaks are very sharp nearly every spectrum must be inspected individually to determine the identity of the component. Later in the chromatographic run when the peaks are broader, only selected scans need to be analyzed.

Identification of resolved components is achieved by comparing the mass cracking patterns of the unknown mass spectra to an eight major peak index of mass spectra (9). Individual difficult unknowns are searched through the use of the Cornell University STIRS and PBM systems. Unknowns are also submitted to the EPA MSSS system for identification. When feasible, the identifications are confirmed by comparing the cracking pattern and elution temperatures for two different chromatographic columns (SE-30 and Carbowax SCOT capillaries) for the unknown and authentic compounds. The relationship between the boiling point of the identified halogenated hydrocarbon and the elution temperature on a non-polar column (the order of elution of constituents is predictable in homologous series since the SE-30 SCOT capillary separates primarily on the basis of boiling point) is carefully considered in making structure assignments.

Mass spectra search programs are operational at the Triangle Universities Computation Center (TUCC). RTI maintains twice daily service to TUCC, which is one-quarter mile distance from the RTI campus. Additional information about each magnetic tape containing the mass spectra of halogenated hydrocarbons is entered directly into the TUCC job stream using a remote job entry processing. This is normally done using one of the five terminals located within the Analytical Sciences Laboratory. The control program contains instructions for processing selected spectra or entire gc runs. The computer program compares simultaneously either the entire library of 25,000 compounds or some subset of this library. The complete report showing the best fits for each of the unknowns is produced at TUCC and printed out at the high speed terminals located on the RTI campus.

8.3.2 Quantitative Analysis

In many cases the estimation of the level of pollutants by capillary gas chromatography in combination with mass spectrometry is not feasible utilizing only the total ion current monitor (see Fig. A-3 for example). Since baseline resolution between peaks is not always achieved, we employ techniques (previously developed under contract) whereby full spectra are obtained during the chromatographic separation step, and then selected ions are presented as mass fragmentograms using computer software programs which allow the possibility of deconvoluting constituents not resolved in the total ion current chromatogram (6). Examples are depicted in Figures A-6 and A-7 which represent an ambient air sample with a TIC profile as in Fig. A-3.

In our GC/MS/COMP system we request (from the Varian 620/L) dedicated computer mass fragmentograms for any combination of m/e ions when full mass spectra are obtained during chromatography; thus selectivity is obtained by selecting the unique ion for that particular organic substance, and this is represented versus time with subsequent use of that ion intensity for quantitation. Also, quantitation with external standards is easily achieved using the intensity of the total ion current monitor or the use of a unique mass cracking ion in the mass spectrum of that external standard. Thus, we use mass fragmentography for the quantitation of organics in ambient air when the total ion current is inadequate due to lack of complete resolution between components.

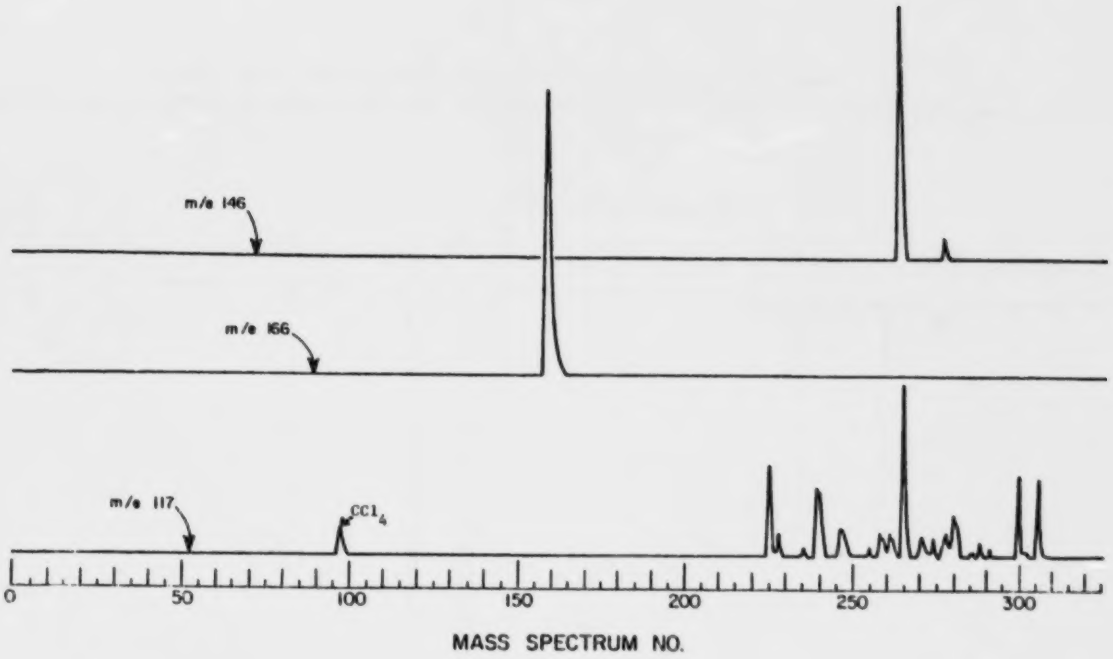


Figure A-6. Mass fragmentograms of characteristic ions representing carbon tetrachloride (m/e 117), tetrachloroethylene (m/e 166) and *m*-dichlorobenzene (m/e 146) in ambient air.

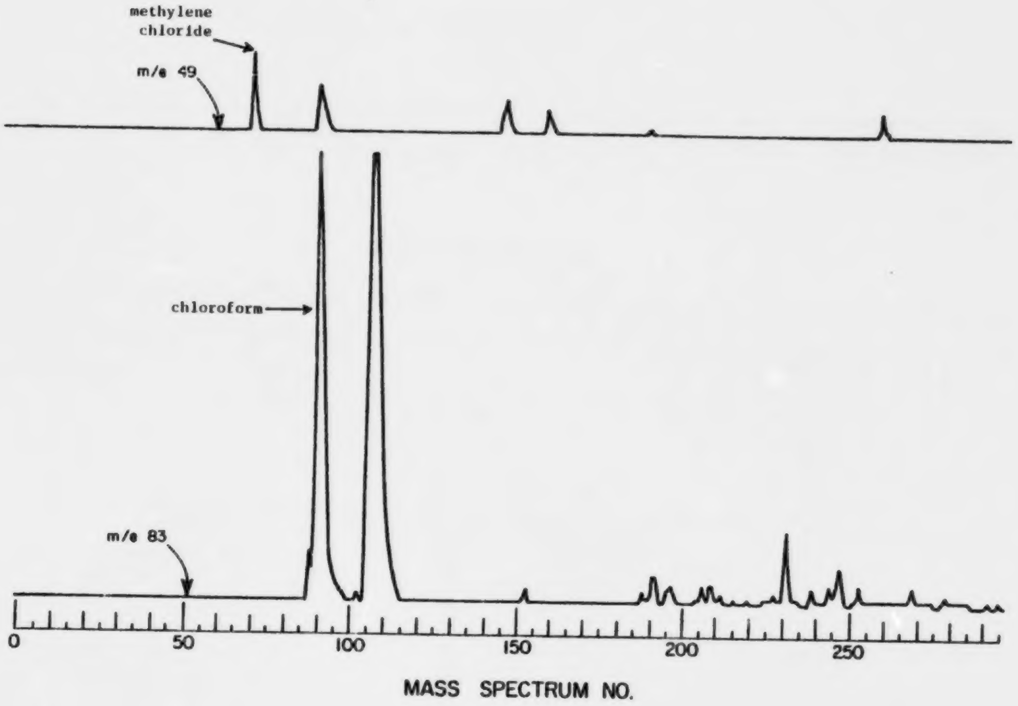


Figure A-7. Mass fragmentograms of characteristic ions representing methylene chloride (m/e 49) and chloroform (m/e 83) in ambient air.

As described previously, the quantitation of constituents in ambient air samples is accomplished either by utilizing the total ion current monitor or, when necessary, mass fragmentograms. In order to eliminate the need to obtain complete calibration curves for each compound to be quantitated, we use the method of relative molar response (RMR) factors (10). Successful use of this method requires information on the exact amount of standard added and the relationship of RMR (unknown) to the RMR (standards). The method of calculation is as follows:

$$(1)\quad \mathrm{RMR}_{\mathrm{unknown/standard}} = \frac{A_{\mathrm{unk}}/\mathrm{Moles}_{\mathrm{unk}}}{A_{\mathrm{std}}/\mathrm{Moles}_{\mathrm{std}}}$$

A = peak area, determined by integration or triangulation.

The value of RMR is determined from at least three independent analysis.

$$(2)\quad \mathrm{RMR}_{\mathrm{unk/std}} = \frac{A_{\mathrm{unk}}/g_{\mathrm{unk}}/\mathrm{GMW}_{\mathrm{unk}}}{A_{\mathrm{std}}/g_{\mathrm{std}}/\mathrm{GMW}_{\mathrm{std}}}$$

A = peak area, as above
g = number of grams present
GMW = gram molecular weight

Thus, in the sample analyzed:

$$(3)\quad g_{\mathrm{unk}} = \frac{A_{\mathrm{unk}}\cdot \mathrm{GMW}_{\mathrm{unk}}\cdot g_{\mathrm{std}}}{A_{\mathrm{std}}\cdot \mathrm{GMW}_{\mathrm{std}}\cdot \mathrm{RMR}_{\mathrm{unk/std}}}$$

The standard can be added as an internal standard during sampling; however, since the volume of air taken to produce a given sample is accurately known, it is also possible and more practical to use an external standard whereby the standard is introduced into the cartridge just prior to its analysis. Two standards, hexafluorobenzene and perfluorotoluene are used for the purpose of calculating RMR's. From previous research, it has been determined that the retention times for these two compounds are such that they elute from the glass capillary column (SE-30) at a temperature and retention time which does not interfere with the analysis of unknown compounds in ambient air samples.

Since the volume of air taken to produce a given sample is accurately known and an external (or internal) standard is added to the sample, then the weight can be determined per cartridge (hence the concentration of the unknown). This approach for quantitating ambient air pollutants requires that the RMR be determined for each constituent of interest. Thus, when an ambient air sample is taken, the external standard is added during the analysis at a known concentration. It is not imperative at this point to know what the RMR of each of the constituents in the sample happens to be; however, after the unknowns are identified, the RMR can be subsequently determined and the unknown concentration calculated in the original sample. In this manner it is possible to obtain qualitative and quantitative information on the same sample with a minimum of effort.

9.0 References

1. Pellizzari, E. D., Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. Publication No. EPA-650/2-74-121, Contract No. 68-02-1228, 148 pp., July, 1974.
2. Pellizzari, E. D., Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. Publication No. EPA-600/2-76-076, Contract No. 68-02-1228, 185 pp., November, 1975.
3. Pellizzari, E. D., J. E. Bunch, B. H. Carpenter and E. Sawicki, Environ. Sci. Tech., 9, 552 (1975).
4. Pellizzari, E. D., B. H. Carpenter, J. E. Bunch and E. Sawicki, Environ. Sci. Tech., 9, 556 (1975).
5. Pellizzari, E. D., The Measurement of Carcinogenic Vapors in Ambient Atmospheres. Publication No. EPA-600/7-77-055, Contract No. 68-02-1228, 288 pp., June, 1977.
6. Pellizzari, E. D., J. E. Bunch, R. E. Berkeley and J. McRae, Anal. Chem., 48, 803 (1976).
7. Pellizzari, E. D., Quarterly Report No. 1, EPA Contract No. 68-02-2262, February, 1976.
8. Pellizzari, E. D., J. E. Bunch, R. E. Berkeley and J. McRae, Anal. Lett., 9, 45 (1976).
9. "Eight Peak Index of Mass Spectra", Vol. 1, (Tables 1 and 2) and II (Table 3), Mass Spectrometry Data Centre, AWRE, Aldermaston, Reading, RF74PR, UF, 1970.

10. Pellizzari, E. D., Quarterly Report No. 3, EPA Contract No. 68-02-2262, in preparation.

Analytical protocol revised 5/31/78.

APPENDIX B

SAMPLING AND ANALYSIS FOR VERY VOLATILE ORGANICS (e.g., METHYL CHLORIDE METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE) IN AMBIENT AIR

APPENDIX B

SAMPLING AND ANALYSIS FOR VERY VOLATILE ORGANICS (E.G., METHYL CHLORIDE, METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE) IN AMBIENT AIR

1.0 Principle of Method

Very volatile compounds (e.g., methyl chloride, methyl bromide, vinyl chloride and vinyl bromide) are concentrated from ambient air on SKC carbon in a short, glass tube (1). Recovery of these volatile halogenated hydrocarbons is accomplished by thermal desorption and purging with helium to transfer the trapped vapors from the carbon cartridge to a Tenax GC cartridge through a calcium sulfate drying tube to remove excessive amounts of water. The vapors are then transferred from Tenax into a liquid nitrogen-cooled nickel capillary trap by thermal desorption and purging with helium (2), and the vapors are introduced onto a high resolution glass, gas chromatographic column where the constituents are separated from each other (2). Identification and quantification of very volatile compounds in the sample are accomplished by mass spectrometry, either by measuring the intensity of the total ion current signal or mass fragmentography (3). The collection and analysis systems are shown in Figure B-1.

2.0 Range and Sensitivity

The linear range of the mass spectrometric signals for organic compounds depends upon two principle features. The first is a function of the breakthrough volume of each specific compound trapped on the SKC carbon sampling cartridge and the second is related to the inherent sensitivity of the mass spectrometer (3,4). Thus, the range and sensitivity is direct function of each compound. The linear range for quantification on the gas chromatograph/mass spectrometry/computer (GC/MS/COMP) is generally over three orders of magnitude. Tables B-1 and B-2 lists the breakthrough volumes for methyl chloride, methyl bromide, vinyl chloride and vinyl bromide on SKC carbon.

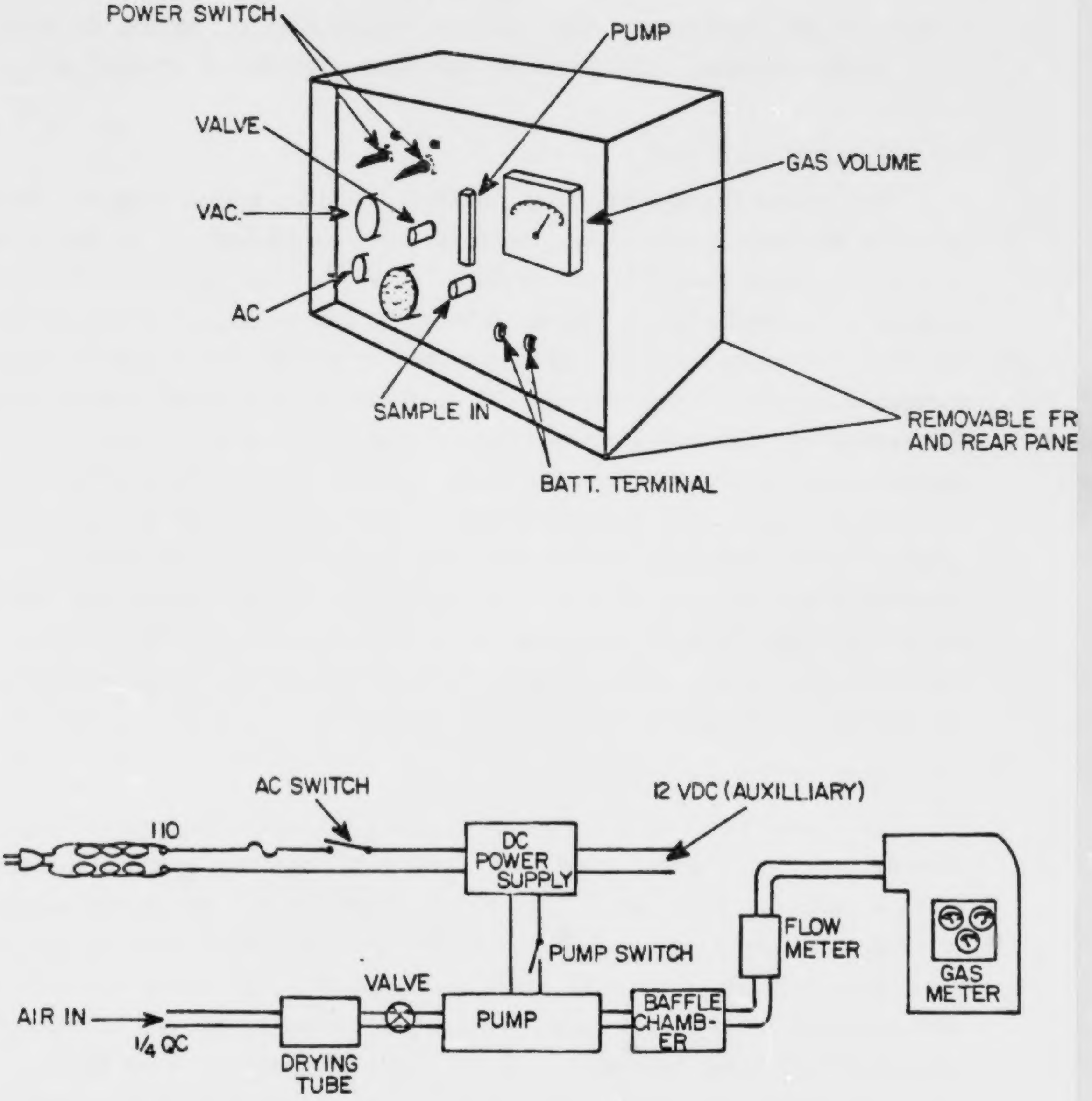

POWER SWITCH
PUMP
VALVE
GAS VOLUME
VAC.
AC
SAMPLE IN
REMOVABLE FR
AND REAR PANE
BATT. TERMINAL
AC SWITCH
12 VDC (AUXILLIARY)
110
DC
POWER
SUPPLY
PUMP SWITCH
FLOW
METER
GAS
METER
VALVE
AIR IN
1/4 QC
PUMP
BAFFLE
CHAMB-
ER
DRYING
TUBE

Figure B-1. Nutech Model 221-A AC-DC Sampler

Table B-1. ESTIMATION OF BREAKTHROUGH VOLUMES FOR VINYL CHLORIDE AND VINYL BROMIDE ON SKC CARBON (104)

Reproduced from best available copy.

Temperature °C (°F)	Vinyl Chloride		Vinyl Bromide	
	ℓ/g	ℓ/2.52 g[a]	ℓ/g	ℓ/2.52 g[a]
10 (50)	104	262	388	978
15.5 (60)	81	204	306	771
21.1 (70)	63	159	241	608
26.7 (80)	49	123	190	479
32.2 (90)	38	96	150	378
37.8 (100)	30	76	118	298

[a] A 1.5 cm i.d. x 4.0 cm bed of carbon weighs 2.52 g.

Table B-2. ESTIMATION OF BREAKTHROUGH VOLUMES FOR METHYL CHLORIDE AND METHYL BROMIDE ON SKI CARBON (104)

Temperature °C (°F)	Methyl Chloride		Methyl Bromide	
	ℓ/g	ℓ/2.52 g	ℓ/g	ℓ/2.52 g
10 (50)	14.3	36	98	248
15.5 (60)	11.1	28	75	188
21.1 (70)	8.7	22	57	143
26.7 (80)	7.5	19	43	108
32.2 (90)	5.6	14	32	82
37.8 (100)	4.4	11	25	62

Table B-3 lists the approximate limits of detection for methyl chloride, methyl bromide, vinyl chloride and vinyl bromide based upon these breakthrough volumes. As it might be expected, the highest sensitivity is observed for vinyl bromide, and the lowest for methyl chloride. Nevertheless, the limits of detection are in the parts per trillion range.

3.0 Interferences

Because of the unique isotopic clusters for chlorine and bromine in these compounds, the background that is generally observed at their retention times on a glass capillary column will not interfer with their qualitative and quantitative analyses.

4.0 Reproducibility

The reproducibility of this method has been determined to be approximately ±20% of the relative standard deviation for the four compounds when replicate samples are examined (3). The reproducibility is a function of several factors. (1) The ability to acurately determine the breakthrough volume for each compound; (2) The accurate measurement of the ambient air volume sampled; (3) The percent recovery of the compound from the carbon sampling cartridge after a period of storage; (4) The reproducibility of thermally recovering each compound from the carbon cartridge and of sample introduction into the analytical system; (5) The accuracy and determination of the relative molar response ratios between the compounds of interest and the external standards used for calibrating the analytical system; (6) The relative efficiency and reproducibility of transferring the trapped vapors from the carbon sampling cartridge to the Tenax GC cartridge prior to analysis in order to remove the excessive amounts of water using calcium chloride; (7) The reproducibility of transmitting the sample through the high resolution gas chromatographic column, and (8) The day-to-day reliability of the ms/comp system (2-4).

The accuracy of analysis is generally ±15% of the amount determined as shown by repeated analysis of the halogenated hydrocarbons. The accuracy of the analysis is dependent upon the storage period.

Table B-3. APPROXIMATE LIMIT OF DETECTION FOR METHYL CHLORIDE, METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE[a]

	Ambient Air Temperature °C (°F)				
	10 (50)	15.5 (60)	21.1 (70)	26.7 (132)	32.2 (90)
Methyl chloride[b]	138 (69)	178 (89)	227 (114)	253 (132)	357 (178)
Methyl bromide[b]	8 (2.1)	11 (2.8)	14 (3.6)	18 (4.8)	24 (6.3)
Vinyl chloride[c]	48 (20)	62 (26)	79 (33)	102 (42)	131 (55)
Vinyl bromide[c]	5 (1.2)	6.5 (1.5)	8.2 (1.9)	10.5 (2.5)	28 (6.7)

[a] Values are in ng/m^3 (ppt)
[b] Estimation of L.O.D. based on 2.52 g carbon
[c] Estimation of L.O.D. based on 1.0 g carbon

5.0 Apparatus

5.1 Sampling Cartridges

The sampling tubes are prepared by packing a 10 cm long x 1.5 cm id glass tube with 2-4 cm of SKC carbon Lot No. 104, with glass wool in the ends to provide support (3,4). The carbon cartridges are conditioned at 400°C with a helium flow of approximately 30 ml/min for 30 min. The conditioned cartridges are transferred to Kimax® culture tubes, immediately sealed using Teflon lined caps, and cooled. This procedure is performed in order to avoid recontamination of the sorbent bed (3,4).

Cartridge samplers with longer beds of sorbents may be prepared using a proportionally increased amount of carbon in order to achieve a larger breakthrough volume for each compound, thus increasing the overall sensitivity of the technique. However, it must be noted that the percent recovery of the organic compounds significantly decreases when the amount of carbon is increased and/or when an excessive length of storage period is employed (more than a week).

5.2 Gas Chromatographic Column

A 0.35 mm i.d. x 100 m glass SCOT capillary column coated with OV-101 stationary phase and 0.1% benzyltriphenylphosphonium chloride is used for effecting resolution. The capillary column is conditioned for 48 hrs at 230°C at 1.5 - 2.0 ml/min of helium flow.

A Finnigan type glass type jet separator on a Varian MAT CH-7 GC/MS/COMP system is employed to interface the glass capillary column to the mass spectrometer. The glass jet separator is maintained at 240°C.

5.3 Inlet-Manifold

An inlet-manifold for thermally recovering compounds of interest trapped on SKC carbon sampling cartridges is employed and is shown in Figure

5.4 Gas Chromatograph

A Varian 1700 gas chromatograph is used to house the glass capillary column and is interfaced to the inlet-manifold (Figure B-1).

5.5 Mass Spectrometry/Computer

A Varian MAT CH-7 mass spectrometer with a resolution of 2000 equipped with single ion monitoring and mass fragmentography capabilities is used in tandem with the gas chromatograph (Figure B-1). The mass spectrometer is interfaced to Varian 620/L computer (Figure B-1).

6.0 Reagents and Materials

SKC carbon Lot No. 104 is from SKC Carbon Company, Boston, MA. All reagents used are analytical reagent grade and distilled in glass prior to use.

7.0 Procedure

7.1 Cleaning of Glassware

All glassware, sampling tubes, cartridge holders, etc. are washed in Isoclean®/water, rinsed with deionized distilled water, acetone and air dried. Glassware is heated to 450-500°C for two hours to insure that all organic material has been removed prior to its use.

7.2 Preparation of Carbon

Virgin carbon is packed into glass sampling tubes without further purification. Used carbon cartridges are not recycled.

7.3 Collection of Very Volatile Compounds in Ambient Air

Continuous sampling of ambient air is accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Figure 1). Flow rates are maintained at 1 ℓ/min using critical orifices and the total flow is monitored through a calibrated rotameter. The total flow is also registered by a dry gas meter. Concomitant with these parameters the temperature is continuously recorded with a Meteorology Research Incorporated weather station since the breakthrough volume is important in order to obtain quantitative data on these compounds. This portable sampling unit operates on a 12-volt storage battery and it is capable of continuous operation up to a period of 24 hours. However, in most cases the sampling period consisted of one to two hours at the rates which were employed in the field. This portable sampling unit is utilized for obtaining "high volume" samples. Duplicate cartridges are deployed on each sampling unit and are in tandem with Tenax GC cartridges. The carbon cartridges serve as a backup to the Tenax GC cartridge for collecting the more highly volatile constituents which have a low breakthrough volume on Tenax GC. A total of four portable sampling units are available for sampling ambient air surrounding the bromine industry.

In addition to the Nutech samplers, five duPont personal samplers are used to sample "low volumes" of ambient air as well as long term integrated samples (12-36 hrs). An identical SKC carbon sampling cartridge is employed in this case and sampling is conducted in duplicate. The flow rate is balanced between duplicate cartridges using critical orifices to maintain a rate of 25 or 100 ml/min per cartridge.

7.4 Analysis of Sample

The conditions for transferring very volatile organic compounds from SKC carbon sampling cartridges to Tenax GC sampling cartridges prior to instrumental analysis is shown in Table B-4. A 1.5 x 2 cm bed of calcium sulfate is used to remove the water vapor prior to retrapping of the component vapors on the Tenax GC sampling cartridge.

The instrumental conditions for the analysis of the volatile components on the sorbent carbon sampling cartridge is shown in Table B-5.

7.4.1 Operation of the MS/Comp System (Figure B-1)

The operation of the ms/comp system is identical to as that described for the Analytical Protocol under Appendix A entitled, "Sampling and Analysis for Volatile Organic Compounds in Ambient Air."

7.4.2 Quantitative Analysis

The procedure for the estimation of the level of very volatile compounds by capillary gas chromatography in combination with mass spectrometry is identical to that described for the analytical protocol entitled, "Sampling and Analysis for Volatile Organics in Ambient Air".

8.0 References

1. Pellizzari, E. D. Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. EPA Contract No. 68-02-1228, EPA-650/2-74-121, July 1974, 148 pp.
2. Pellizzari, E. D. Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. EPA Contract No. 68-02-1228, EPA-600/2-75-076, November 1975, 187 pp.

Table B-4. PARAMETERS FOR REMOVING WATER AND TRANSFERRING VAPORS TO TENAX GC

Parameters	Condition
Inlet-manifold	
desorption chamber	295°C
valve	200°C
$CaSO_4$ drying tube (1.5 x 2.0 cm)	ambient temperature
transfer line	ambient temperature
Tenax GC cartridge (1.5 x 6.0 cm)	ambient temperature
Desorption time	10 minutes
He purge rate	10 ml/min

Table B-5. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC	
100 m glass SCOT-OV-101	20-240°C, 4/C° min
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	*m/e* 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 µA
multiplier	6.0
ion source vacuum	~4 x 10^{-6} torr

3. Pellizzari, E. D. Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. EPA Contract No. 68-02-1228, 1976, in preparation.

4. Pellizzari, E. D. Identification of Atmospheric Pollutants by the Combined Techniques of Gas Chromatography/Mass Spectrometry. EPA Contract No. 68-02-2262, 1976, in preparation.

Analytical protocol revised 1/31/77.

APPENDIX C

VOLATILE AND VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AIR IN THE KANAWHA VALLEY, WV

Table C-1. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L2).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	55	C_5H_8 isomer
2B	55	*n*-butane
3	57	acetaldehyde
3A	60	isopentane
4	61	acetone
4A	62	furan (tent.)
4B	64	vinylidene chloride (tent.)
5	65	methylene chloride
6A	67	CS_2
7	69	C_4H_8O isomer
7A	71	methyl vinyl ketone (tent.)
8	72	2-methylpentane
8A	74	C_4H_8O isomer
9	75	3-methylpentane
10	76	hexafluorobenzene (eS)
11	77	*n*-hexane
11A	78	chloroform
12	82	perfluorotoluene (eS)
12A	83	methylcyclopentane
13	88	benzene
13A	89	cyclohexane
13B	94	*n*-pentanal
14	97	*n*-heptane + acetic acid
15	109	toluene
16	148	benzaldehyde
17	151	phenol
17A	151	$C_{11}H_{24}$ isomer
18	165	acetophenone

Table C-2. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L2)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2A	54	C_4H_8 isomer
3	55	acetaldehyde + *n*-butane (tent.)
3A	55	C_4H_8 isomer
3B	59	isopentane
4	61	acetone
4A	61	C_5H_{10} isomer
4B	62	*n*-pentane
4D	64	methylene chloride
5B	70	C_4H_6O isomer
6	71	2-methylpentane
6A	72	methyl isopropyl ketone
6B	73	butanal (tent.)
7	74	3-methylpentane
8	75	hexafluorobenzene (eI)
8A	76	*n*-hexane
9	77	chloroform
10	81	perfluorotoluene (eI)
10A	82	methylcyclopentane
10B	83	1,2-dichloroethane (tent.)
11	84	1,1,1-trichloroethane
11A	86	C_6H_8 isomer
12	87	benzene
12A	88	carbon tetrachloride
12B	89	cyclohexane
13	90	2-methylhexane
13A	91	acetic acid
14	92	3-methylhexane
14A	93	C_7H_{14} isomer
15	94	C_7H_{14} + $C_5H_{10}O$ isomers
16	95	trichloroethylene
16A	96	C_7H_{14} isomer
17	97	*n*-heptane
17A	98	C_7H_{14} isomer
18	101	methylcyclohexane
18A	102	4-methyl-2-pentanone
19	103	C_8H_{18} isomer
20	108	C_8H_{16} isomer (tent.)
21	109	toluene
22	110	C_8H_{18} isomer
22A	111	C_8H_{18} isomer
23	112	C_8H_{18} isomer
23A	113	C_8H_{16} isomer
24	114	C_6H_{12} isomer
24A	115	C_8H_{16} isomer
24B	116	C_8H_{16} isomer
25	117	*n*-octane
26	118	tetrachloroethylene
26A	120	C_9H_{20} isomer (tent.)
27	121	$C_7H_{14}O$ isomer
28	122	C_8H_{16} isomer
29	123	C_9H_{20} isomer
29A	124	C_9H_{20} isomer
30	125	ethylcyclohexane
30A	125	C_9H_{20} isomer
30B	126	C_9H_{18} isomer
31	128	ethylbenzene
32	130	xylene isomer
32A	130	C_9H_{20} isomer
32B	131	C_9H_{18} isomer
33	132	C_9H_{20} isomer
34	133	C_9H_{20} isomer
35	134	styrene
35A	134	*n*-heptanal (tent.)
36	135	*o*-xylene
36A	136	C_9H_{18} isomer
37	137	*n*-nonane
37A	138	C_9H_{18} isomer
38	140	C_9H_{18} isomer
39	141	isopropylbenzene + $C_{10}H_{22}$ isomers
39A	142	$C_{10}H_{22}$ isomer
40	142	C_9H_{16} isomer
40A	143	$C_{10}H_{22}$ isomer
40B	144	C_3-alkyl cyclohexane isomer
41	144	$C_{10}H_{22}$ isomer
41A	145	$C_{10}H_{20}$ isomer
41B	146	$C_{10}H_{22}$ isomer
42	146	benzaldehyde
42A	146	$C_{10}H_{20}$ isomer
43	147	*n*-propylbenzene
44	148	ethyltoluene isomer
44A	148	$C_{10}H_{22}$ isomer
44B	149	$C_{10}H_{22}$ isomer + phenol
45	150	1,3,5-trimethylbenzene
45A	150	$C_{10}H_{20}$ isomer
46	151	$C_{10}H_{22}$ isomer
47	152	*o*-ethyltoluene
48	153	$C_{10}H_{20}$ isomer
48A	153	$C_{10}H_{18}$ isomer

(continued)

Table C-2. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
49	154	$C_{10}H_{20}$ isomer + *n*-octanal (tent.)
50	154	1,2,4-trimethylbenzene
50A	155	$C_{10}H_{20}$ isomer
51	156	*n*-decane
52	157	dichlorobenzene isomer
52A	157	$C_{10}H_{20}$ isomer
52B	148	C_4-alkyl benzene isomer
52C	148	$C_{11}H_{22}$ isomer
53	149	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
54	160	1,2,3-trimethylbenzene
55	160	$C_{11}H_{24}$ isomer
56	161	$C_{11}H_{22}$ isomer
56A	162	$C_{10}H_{16}$ isomer
56B	162	indan
56C	162	$C_{11}H_{24}$ isomer
57	163	C_4-alkyl cyclohexane isomer
57A	163	$C_{11}H_{22}$ isomer
57B	164	C_4-alkyl benzene isomer
58	164	C_4-alkyl benzene isomer
59	165	acetophenone
59A	165	C_4-alkyl benzene isomer
59B	166	$C_{11}H_{22}$ isomer
60	166	$C_{11}H_{24}$ isomer
61	167	$C_{11}H_{24}$ isomer
62	167	C_4-alkyl benzene isomer
62A	168	$C_{10}H_{18}$ isomer
62B	168	$C_{11}H_{24}$ isomer
63	169	C_4-alkyl benzene isomer
63A	170	$C_{11}H_{22}$ isomer
64	170	C_4-alkyl benzene isomer
65	171	C_4H_7-benzene + $C_{11}H_{22}$ isomers
65A	171	C_4-alkyl benzene isomer
65B	172	$C_{11}H_{22}$ isomer
66	173	*n*-undecane
66A	173	C_5-alkyl benzene isomer
67	176	C_4-alkyl benzene isomer
67A	174	C_5-alkyl benzene isomer
67B	175	$C_{11}H_{22}$ isomer
68	176	tetramethylbenzene isomer
69	177	C_4-alkyl benzene isomer
69A	178	C_2-alkyl phenol isomer
70	179	C_5-alkyl benzene isomer
71	180	C_5-alkyl benzene + C_4H_7-benzene isomers
71A	180	$C_{12}H_{24}$ isomer
71B	181	$C_{11}H_{20}$ isomer
71C	181	C_5-alkyl benzene isomer
71D	181	C_2-alkyl phenol isomer
71E	182	C_4H_7-benzene isomer
72	182	C_4-alkyl benzene isomer
73	183	C_5-alkyl benzene isomer
74	184	1,2,3,4-tetrahydronaphthalene
74A	184	C_5-alkyl benzene + $C_{13}H_{28}$ isomers
75	185	C_5-alkyl benzene isomer
75A	186	$C_{10}H_{16}$ + $C_{13}H_{26}$ isomers
75B	186	$C_{12}H_{24}$ isomer
76	187	naphthalene
76A	188	$C_{12}H_{24}$ isomer
76B	189	C_5-alkyl benzene isomer
77	189	*n*-dodecane
78	191	C_5-alkyl benzene isomer
79	192	$C_{13}H_{28}$ isomer
80	193	C_6-alkyl benzene isomer (tent.)
80A	194	$C_{13}H_{26}$ isomer
81	195	$C_{13}H_{28}$ isomer
81A	195	C_5-alkyl benzene isomer
81B	197	$C_{13}H_{28}$ isomer
82	198	C_5H_9-benzene isomer
82A	198	C_6-alkyl benzene isomer
83	199	$C_{13}H_{26}$ isomer (tent.)
85	203	$C_{13}H_{26}$ isomer
86	204	*n*-tridecane
86A	205	β-methylnaphthalene
86B	206	$C_{13}H_{26}$ isomer
87	207	α-methylnaphthalene
88	211	sat. hydrocarbon (tent.)
89	213	$C_{14}H_{30}$ isomer
90	214	alkyl butyrate
90A	215	biphenyl
90B	216	$C_{14}H_{28}$ isomer
90C	217	diphenyl ether or $C_{12}H_{10}O$ isomer
91	218	*n*-tetradecane
91A	220	dimethylnaphthalene isomer
92	223	dimethylnaphthalene isomer
93	226	$C_{15}H_{32}$ isomer (tent.)
93A	227	$C_{15}H_{30}$ isomer
94	230	*n*-pentadecane

(continued)

Table C-2. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
95	233	unknown	100	240	n-heptadecane
96	239	diethyl phthalate	101	240	unsat. hydrocarbon
99	240	unsat. hydrocarbon	102	240	sat. hydrocarbon

Table C-3. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L5).

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2	14	68	3-methylpentane
4	52	n-propane (tent.)	15	70	hexafluorobenzene (es)
4A	53	butene isomer	16	71	n-hexane
5	53	n-butane	16A	72	chloroform
5A	54	butene (tent.)	17	75	perfluorotoluene (es)
6	55	acetaldehyde	18	76	methylcyclopentane
7	57	isopentane	18A	77	C_6H_{10} isomer
8	58	acetone	18B	78	benzene
9	59	n-pentane	18C	79	carbon tetrachloride
9A	60	diethyl ether	18D	80	cyclohexane
10	61	vinylidene chloride	19	103	toluene
10A	61	methylene chloride	19A	107	acetic acid (tent.)
12	63	CS_2	20	145	phenol
13	66	2-methylpentane	20A	146	$C_{11}H_{24}$ isomer
13A	68	n-butanal			

Table C-4. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L5).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	54	propane
2B	55	butane
2C	55	acetaldehyde
2D	60	dimethyl ether
2E	60	isopentane
3	61	acetone
3A	65	vinylidene chloride
4	66	dichloromethane
6	74	2-methylpentane
6A	75	C_6H_{12} isomer
6B	76	3-methylpentane
7	78	hexafluorobenzene (eS)
8	79	*n*-hexane
8A	80	chloroform
8B	81	C_4H_8O isomer
8C	82	ethyl acetate
9	83	perfluorotoluene (eS)
9A	84	methylcyclopentane
9B	86	1,1,1-trichloroethane
9C	88	C_6H_{10} isomer
10	89	benzene
10A	90	carbon tetrachloride
10B	91	acetic acid (tent.)
11	91	C_7H_{16} isomer
12	93	C_7H_{16} isomer
13	95	C_7H_{14} isomer
13A	96	trichloroethylene (tent.)
14	96	C_8H_{18} isomer
15	98	*n*-heptane
16	102	methylcyclohexane
17	104	C_8H_{18} + $C_7H_{14}O$ isomer
18	109	toluene
19	110	C_8H_{18} isomer
20	112	C_8H_{18} isomer
20A	113	C_8H_{16} isomer
20B	114	hexanal (tent.)
20C	115	C_8H_{16} isomer
21	117	*n*-octane
22	118	tetrachloroethylene
22A	122	C_8H_{16} isomer
22B	123	C_9H_{20} isomer
23	125	C_9H_{20} isomer (tent.)
24	128	ethylbenzene
25	130	xylene isomer
25A	130	C_9H_{20} isomer
26	132	C_9H_{20} isomer
26A	133	$C_7H_{14}O$ isomer (tent.)
26B	133	styrene
27	134	*o*-xylene
27A	135	C_9H_{18} isomer
28	137	*n*-nonane
28A	140	C_9H_{18} isomer
29	140	isopropylbenzene
30	142	$C_{10}H_{22}$ isomer
31	143	$C_{10}H_{22}$ isomer
31A	144	C_3-alkyl cyclohexane isomer
31B	145	$C_{10}H_{22}$ isomer
32	145	benzaldehyde
33	146	*n*-propylbenzene + $C_{10}H_{20}$ isomer
34	147	ethyltoluene isomer
34A	148	$C_{10}H_{22}$ isomer + phenol
35	149	1,3,5-trimethylbenzene + $C_{11}H_{24}$ isomer
36	150	$C_{10}H_{22}$ isomer
36A	151	*o*-ethyltoluene
37	151	$C_{10}H_{22}$ isomer
37A	152	$C_{10}H_{20}$ isomer
38	153	*n*-octanal
39	153	1,2,4-trimethylbenzene
39A	154	$C_{10}H_{20}$ isomer
40	155	*n*-decane
41	156	dichlorobenzene isomer
41A	157	C_4-alkyl benzene isomer
41B	158	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
42	159	1,2,3-trimethylbenzene
43	159	$C_{11}H_{24}$ isomer
43A	160	$C_8H_{16}O$ isomer
44	160	$C_{11}H_{24}$ isomer
44A	161	indan
44B	162	$C_{11}H_{22}$ isomer
45	162	C_4-alkyl cyclohexane isomer
46	163	C_4-alkyl benzene isomer
47	164	acetophenone
47A	165	C_4-alkyl benzene isomer
48	165	$C_{12}H_{24}$ isomer
49	166	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
50	168	C_4-alkyl benzene isomer
50A	169	$C_{11}H_{22}$ isomer

(continued)

Table C-4. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
51	169	C_4-alkyl benzene isomer
52	170	*n*-nonanal
52A	171	$C_{11}H_{22}$ isomer
53	172	*n*-undecane
53A	173	C_4-alkyl benzene isomer
53B	174	$C_{11}H_{22}$ isomer
54	175	C_4-alkyl benzene isomer
55	177	C_2-alkyl phenol isomer
55A	178	C_5-alkyl benzene isomer
55B	178	$C_{12}H_{24}$ isomer
55C	179	C_4H_7-benzene isomer
55D	179	C_5-alkyl cyclohexane isomer
56	180	C_2-alkyl phenol isomer
56A	181	C_4H_7-benzene isomer
56B	181	C_4-alkyl benzene isomer
56C	183	C_5-alkyl benzene isomer
56D	184	$C_{12}H_{26}$ + C_5-alkyl benzene isomers
56E	185	C_3-alkyl phenol isomer
57	186	naphthalene
57A	187	*n*-decanal
57B	187	$C_{12}H_{24}$ isomer
57C	188	C_5-alkyl benzene isomer
58	188	*n*-dodecane
58A	189	C_5-alkyl benzene isomer
58B	190	$C_{13}H_{26}$ isomer
58C	190	C_3-alkyl phenol isomer
58D	191	$C_{13}H_{28}$ isomer
59A	195	unsaturated hydrocarbon
59B	199	saturated hydrocarbon
59C	201	$C_{11}H_{22}O$ isomer
59D	201	*n*-undecanal (tent.)
60	202	*n*-tridecane
60A	203	β-methylnaphthalene
61	205	α-methylnaphthalene
62	211	alkyl butyrate (tent.)
63	212	alkyl butyrate (tent.)
64	213	biphenyl
64A	215	$C_{14}H_{28}$ isomer (tent.)
65	216	*n*-tetradecane + diphenyl ether (tent.)
65A	220	C_2-alkyl naphthalene (tent.)
66	225	saturated hydrocarbon
66A	228	$C_{15}H_{30}$ isomer (tent.)
67	229	*n*-pentadecane
68	231	unknown
71	240	$C_{17}H_{36}$ isomer
72	240	*n*-heptadecane

Table C-5. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L6).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2	11A	66	C_5H_{10} isomer (tent.)
3	53	propane	12	67	2-methylpentane
3A	53	C_4H_8 isomer	13	70	3-methylpentane
4	54	_n_-butane	14	71	hexafluorobenzene (eI)
4A	55	butene isomer	15	72	_n_-hexane
4B	55	acetaldehyde	15A	73	chloroform
5	57	isopentane	16	76	perfluorobenzene (eI)
7	58	acetone	17	77	methylcyclopentane
8	59	_n_-pentane	17A	79	1,1,1-trichloroethane (tent.)
8A	59	C_5H_{10} isomer	17B	82	benzene
8B	60	vinylidene chloride	17C	84	cyclohexane
9	61	methylene chloride	17E	96	methylcyclohexane
11	63	CS_2	18	104	toluene

Table C-6. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L6).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	53	propane
2B	54	C_4H_8 isomer
2C	54	n-butane
2D	56	acetaldehyde
2E	59	dimethyl ether
3	60	acetone
3B	63	diethyl ether
4	64	vinylidene chloride
5	65	dichloromethane
6A	70	C_4H_6O isomer (tent.)
7	71	2-methylpentane
8	74	3-methylpentane
8A	74	n-butanal
8B	75	C_6H_{12} isomer
9	75	hexafluorobenzene (eI)
10	76	n-hexane
10A	77	chloroform
10B	78	methyl ethyl ketone
11	79	ethyl acetate
11A	80	C_6H_{12} isomer
12	81	perfluorotoluene (eI)
13	82	methylcyclopentane
14	83	1,1,1-trichloroethane
15	86	benzene
15A	88	cyclohexane
16	89	2-methylhexane
16A	90	2,3-dimethylpentane
17	91	3-methylhexane
18	93	C_7H_{14} isomer
19	94	trichloroethylene (tent.) + C_8H_{18} isomer
19A	95	acetic acid
20	96	n-heptane
20A	97	C_7H_{14} isomer
21	101	methylcyclohexane
22	103	C_8H_{18} isomer
23	105	C_8H_{16} isomer
24	107	C_8H_{18} isomer
25	108	toluene
26	109	C_8H_{18} isomer
26A	110	C_8H_{16} isomer
27	111	C_8H_{18} isomer
28	113	C_8H_{16} isomer
28A	114	C_8H_{18} isomer
28B	114	$C_6H_{12}O$ isomer
28C	115	C_8H_{16} isomer
29	115	C_8H_{16} isomer
30	116	n-octane
30A	117	C_8H_{16} isomer
31	118	tetrachloroethylene
32	120	C_9H_{20} isomer
33	121	C_9H_{20} isomer
34	123	C_9H_{20} isomer
34A	123	C_9H_{18} isomer
35	124	C_9H_{20} isomer
35A	125	C_9H_{18} isomer
36	128	ethylbenzene
36A	128	C_9H_{18} isomer
37	129	xylene isomer
37A	130	C_9H_{20} isomer
38	131	C_9H_{20} isomer
38A	132	$C_7H_{14}O$ isomer (tent.)
39	133	styrene
40	134	o-xylene
40A	135	C_9H_{18} isomer
41	136	n-nonane
41A	138	$C_{10}H_{20}$ isomer
42	139	C_9H_{18} isomer
43	140	isopropylbenzene + $C_{10}H_{22}$ isomer
44	141	C_9H_{16} isomer
44A	142	$C_7H_{14}O$ isomer (tent.)
45	143	$C_{10}H_{22}$ isomer
45A	144	C_3-alkyl cyclohexane isomer
45B	145	$C_{10}H_{20}$ isomer
46	145	benzaldehyde
47	146	n-propylbenzene
48	147	ethyltoluene isomer
48A	148	$C_{10}H_{22}$ isomer
49	149	1,3,5-trimethylbenzene
49A	150	$C_{10}H_{20}$ isomer
50	150	$C_{10}H_{22}$ isomer
51	151	o-ethyltoluene
52	152	$C_{10}H_{20}$ isomer
52A	153	$C_{10}H_{20}$ isomer
53	153	n-octanal + methylstyrene isomer (tent.)
54	154	1,2,4-trimethylbenzene
54A	153	$C_{10}H_{20}$ isomer
55	155	n-decane
55A	156	$C_{10}H_{20}$ isomer

(continued)

Table C-6. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
56	156	C_4-alkyl benzene isomer
57	158	$C_{11}H_{24}$ isomer
57A	158	C_4-alkyl benzene isomer
58	159	1,2,3-trimethylbenzene
59	160	$C_{11}H_{24}$ isomer
60	161	$C_{11}H_{24}$ + dichlorobenzene isomers (tent.)
60A	161	indan + $C_{11}H_{22}$ isomer
61	162	C_4-alkyl cyclohexane isomer
61A	163	C_4-alkyl benzene isomer
62	163	C_4-alkyl benzene isomer
62A	163	$C_{11}H_{24}$ isomer
63	164	C_4-alkyl benzene isomer + acetophenone
63A	164	*n*-butylbenzene
64	165	$C_{11}H_{22}$ isomer
65	165	$C_{11}H_{24}$ isomer
66	166	C_4-alkyl benzene isomer
66A	166	$C_{11}H_{22}$ isomer
66B	167	$C_{10}H_{18}$ isomer
67	167	$C_{11}H_{24}$ isomer
67A	168	C_4-alkyl benzene isomer
67B	168	$C_{11}H_{22}$ isomer
68	169	C_4-alkyl benzene isomer
69	170	$C_{11}H_{22}$ isomer
70	171	*n*-nonanal
71	172	*n*-undecane
71A	173	C_4-alkyl benzene isomer
72	174	$C_{11}H_{22}$ isomer
73	176	C_4-alkyl benzene + $C_{12}H_{26}$ isomers
74	177	$C_{12}H_{24}$ isomer
74A	178	C_5-alkyl benzene + C_2-alkyl phenol isomers (tent.)
74B	179	C_4-benzene + C_5-alkyl benzene isomers
75	179	C_5-alkyl cyclohexane isomer
75A	180	$C_{12}H_{24}$ isomer
75B	180	C_5-alkyl benzene isomer
76	181	C_4H_7-benzene isomer
76A	181	C_4-alkyl benzene isomer
76B	182	C_5-alkyl benzene isomer
77	183	$C_{12}H_{26}$ isomer
77A	184	$C_{12}H_{26}$ isomer
77B	184	C_5-alkyl benzene isomer
78	186	naphathalene
78A	187	$C_{12}H_{24}$ isomer
79	188	3-dodecane
79A	189	C_5-alkyl benzene isomer
79B	195	$C_{12}H_{24}$ isomer
80	199	sat. hydrocarbon
80A	202	$C_{13}H_{26}$ isomer
81	203	*n*-tridecane
81A	204	β-methylnaphthalene
81B	204	$C_{13}H_{26}$ isomer
82	206	α-methylnaphthalene
82A	208	$C_{13}H_{26}$ isomer
83	211	C_7-alkyl cyclohexane or $C_{13}H_{26}$ isomer
84	212	alkyl butyrate
85	213	alkyl butyrate
86	217	*n*-tetradecane
86A	219	C_2-alkyl naphthalene isomer
86B	221	C_2-alkyl naphthalene isomer
86C	225	$C_{15}H_{30}$ isomer
88	229	*n*-pentadecane
89	232	unknown
89A	237	$C_{16}H_{32}$ isomer
90	238	diethyl phthalate
91A	240	*n*-hexadecane

Table C-7. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L3).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2	24	86	2,3-dimethylpentane
3A	53	C_4H_8 isomer	24A	86	alkyl ether (tent.)
4	54	acetaldehyde	25	87	3-methylhexane
4A	54	n-butane	26	88	3-pentanone
4B	55	methyl formate (tent.)	26A	89	C_7H_{14} isomer
5	58	isopentane	27	90	1,1,1-trichloroethylene
5A	58	dimethyl ether (tent.)	27A	91	C_7H_{14} isomer
6	59	acetone	28	92	n-heptane
6A	59	furan (tent.)	28A	92	n-propyl acetate
6B	60	C_5H_{10} isomer	28B	93	C_7H_{14} isomer
7	60	n-pentane	29	94	C_7H_{14} isomer
8	61	C_5H_{10} isomer	30	97	methylcyclohexane
8A	62	isopropanol (tent.)	30A	98	4-methyl-2-pentanone
8B	62	C_5H_{10} isomer	31	98	C_8H_{18} isomer
8C	62	methylene chloride	32	99	C_8H_{18} isomer
9	63	methyl acetate	33	101	C_8H_{16} isomer
9B	64	carbon disulfide	33A	102	2-ethylbutanal
10	66	2-methylpropanal	34	103	C_8H_{18} isomer
10A	67	C_6H_{12} isomer	34A	104	C_8H_{16} isomer
10B	68	C_4H_6O isomer	35	104	toluene
11	68	2-methylpentane	36	106	C_8H_{18} isomer
11A	69	methyl isopropyl ketone (tent.)	36A	107	alkyl ether (tent.)
			37	107	C_8H_{18} isomer
12	70	3-methylpentane	37A	109	dimethylcyclohexane isomer
13	71	methyl ethyl ketone	38	109	C_8H_{18} isomer (tent.)
13A	71	C_6H_{12} isomer	38A	110	1,2-dibromoethane (tent.)
14	72	hexafluorobenzene (eI)	38B	111	alcohol isomer (tent.)
15	73	n-hexane	39	112	C_8H_{16} isomer
15A	73	isopropyl ether	40	113	n-octane
15B	74	chloroform	40A	113	n-butyl acetate
15C	74	C_6H_{12} isomer	41	114	tetrachloroethylene
16	75	ethyl acetate	41A	115	C_8H_{16} isomer
16A	75	C_6H_{12} isomer	42	117	C_9H_{20} isomer
16B	76	C_6H_{12} isomer	43	118	C_9H_{20} isomer
17	77	perfluorotoluene (eI)	44	119	C_9H_{20} isomer
18	78	methylcyclopentane	44A	120	C_8H_{16} isomer
18A	79	1,2-dichloroethane (tent.)	44B	120	C_9H_{18} isomer
18B	79	1,1,1-trichloroethane	45	121	C_9H_{20} isomer
19	80	unknown	45A	122	C_9H_{18} isomer
19A	82	C_6H_{10} isomer	45B	123	C_9H_{18} isomer
20	82	isopropyl acetate	46	124	ethylbenzene
20A	83	benzene	46A	124	C_9H_{18} isomer
21	83	carbon tetrachloride	47	126	xylene isomer
22	84	isopropenyl acetate + hexane	47A	126	C_9H_{20} isomer
			48	128	C_9H_{20} isomer
23	85	2-methylhexane	49	129	$C_7H_{14}O$ isomer (tent.)

(continued)

Table C-7. (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
50	130	styrene
50A	130	heptanal
51	131	*o*-xylene
52	132	C_9H_{18} isomer
53	133	cyclohexyl acetate or C_6H_{11} acetate isomer
54	133	*n*-nonane
54A	134	$C_{10}H_{20}$ isomer
55	136	C_9H_{18} isomer
55A	137	$C_{10}H_{22}$ isomer
56	137	isopropylbenzene
56A	137	$C_{10}H_{22}$ isomer
56B	138	$C_{10}H_{20}$ isomer
57	139	C_9H_{16} + $C_{10}H_{22}$ isomer
57A	140	$C_{10}H_{20}$ isomer
58	140	C_3-alkyl cyclohexane + $C_{10}H_{22}$ isomers
58A	141	$C_{10}H_{22}$ isomer
59	141	$C_{10}H_{16}$ + $C_8H_{16}O$ isomers
59A	142	$C_{10}H_{22}$ isomer
60	142	benzaldehyde
60A	142	$C_{10}H_{20}$ isomer
61	142	*n*-propylbenzene
61A	143	$C_{10}H_{20}$ isomer
62	144	ethyltoluene isomer
62A	145	$C_{10}H_{22}$ isomer
62B	145	phenol (tent.)
63	146	1,3,5-trimethylbenzene
63A	146	$C_{10}H_{20}$ isomer
64	147	$C_{10}H_{22}$ isomer
65	148	*o*-ethyltoluene
65A	148	$C_{10}H_{18}$ + $C_{11}H_{24}$ isomers
66	149	$C_{10}H_{20}$ isomer
66A	149	$C_{10}H_{18}$ isomer
67	150	$C_{10}H_{22}$ isomer
67A	150	C_3H_5-benzene isomer
68	151	1,2,4-trimethylbenzene
68A	152	$C_{10}H_{20}$ isomer
69	152	*n*-decane
69A	153	dichlorobenzene isomer
70	153	$C_{10}H_{20}$ isomer + isobutylbenzene
70A	154	sec-butylbenzene
70B	155	$C_{11}H_{22}$ isomer
71	155	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
72	156	1,2,3-trimethylbenzene
73	156	$C_{11}H_{24}$ isomer
74	157	dichlorobenzene + $C_{11}H_{24}$ isomers
74A	158	indan + $C_{10}H_{20}$ isomer
74B	158	$C_{11}H_{24}$ isomer
75	159	C_4-alkyl cyclohexane isomer
75A	159	C_4-alkyl benzene isomer
76	160	propyltoluene isomer
77	161	C_4-alkyl benzene isomer
78	162	$C_{11}H_{24}$ isomer
78A	162	$C_{11}H_{22}$ isomer
79	163	$C_{11}H_{24}$ isomer
80	163	C_4-alkyl benzene isomer
80A	164	$C_{10}H_{18}$ isomer
81	164	$C_{11}H_{24}$ isomer
81A	165	C_4-alkyl benzene isomer
81B	166	C_4H_7-benzene + $C_{11}H_{22}$ isomers
82	167	C_4-alkyl benzene isomer
83	167	C_4H_7-benzene + $C_{11}H_{22}$ isomers
83A	168	$C_{11}H_{22}$ isomer
84	169	*n*-undecane
85	170	C_4-alkyl benzene isomer
85A	170	$C_{11}H_{22}$ isomer
85B	171	C_4-alkyl benzene isomer
85C	171	$C_{12}H_{26}$ isomer
86	172	tetramethylbenzene + $C_{12}H_{26}$ isomers
87	173	C_4-alkyl benzene isomer
87A	174	$C_{11}H_{20}$ isomer
88	174	$C_{12}H_{26}$ + C_2-alkyl phenol isomers
89	175	C_5-alkyl benzene isomer
89A	175	$C_{12}H_{24}$ isomer
90	176	C_5-alkyl benzene + C_4H_7-benzene isomers
91	176	C_5-alkyl cyclohexane isomer
91A	177	$C_{11}H_{20}$ + $C_{12}H_{24}$ isomers
91B	177	C_2-alkyl phenol isomer
92	177	C_4H_7-benzene + C_5-alkyl benzene isomers
93	178	C_4-alkyl benzene isomer
93A	178	$C_{12}H_{26}$ isomer
94	179	C_5-alkyl benzene isomer
95	180	1,2,3,4-tetrahydronaphthalene + C_5-alkyl benzene isomer

(continued)

Table C-7. (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
95A	180	$C_{12}H_{24}$ isomer
96	181	C_5-alkyl benzene isomer
96A	182	$C_{12}H_{24}$ isomer
96B	182	C_6-alkyl benzene isomer
96C	183	C_5H_9-benzene + $C_{12}H_{24}$ isomers
97	183	naphthalene
97A	184	C_5-alkyl benzene isomer
97B	184	C_5-alkyl benzene + $C_{12}H_{24}$ isomers
98	185	*n*-dodecane
99	186	C_5-alkyl benzene + $C_{12}H_{24}$ isomers
100	187	$C_{13}H_{28}$ isomer
101	188	C_6-alkyl benzene isomer
101A	189	$C_{13}H_{28}$ isomer
101B	190	$C_{13}H_{26}$ isomer
102	190	C_6-alkyl benzene isomer
102A	191	$C_{13}H_{26}$ isomer
103	192	C_6-alkyl cyclohexane isomer
103A	193	C_5-alkyl benzene isomer
104	193	$C_{13}H_{28}$ isomer
104A	193	C_5H_9-benzene isomer
105	194	C_6-alkyl benzene isomer
106	195	$C_{13}H_{28}$ isomer
107	196	$C_{14}H_{30}$ isomer
107A	198	$C_{13}H_{26}$ isomer
108	200	*n*-tridecane
108A	200	β-methylnaphthalene
108B	202	C_5-alkyl benzene isomer
109	203	α-methylnaphthalene
109A	204	$C_{14}H_{28}$ isomer
109B	206	$C_{14}H_{28}$ isomer
110	207	$C_{14}H_{30}$ isomer
110A	207	C_6-alkyl benzene isomer
110B	208	$C_{13}H_{26}$ isomer
111	209	$C_{14}H_{30}$ isomer
112	210	alkyl butyrate
113	211	$C_{15}H_{32}$ isomer
113A	211	biphenyl
113B	212	$C_{14}H_{28}$ isomer
114	213	*n*-tetradecane
114A	214	C_2-alkyl naphthalene isomer
115	216	C_2-alkyl naphthalene isomer
115A	217	$C_{15}H_{30}$ isomer
116	218	dimethylnaphthalene isomer
116A	219	$C_{15}H_{30}$ isomer
116B	219	$C_{15}H_{32}$ isomer
117	220	C_2-alkyl naphthalene isomer
118	222	$C_{16}H_{34}$ isomer
119	224	$C_{13}H_{26}O$ isomer (tent.)
120	225	$C_{15}H_{30}$ isomer
121	226	*n*-pentadecane
122	228	unknown
122A	233	$C_{16}H_{34}$ + C_3-alkyl naphthalene isomers
122B	234	unsat. hydrocarbon
123	235	diethyl phthalate (BKG)
123A	237	$C_{14}H_{28}O$ isomer
123B	238	$C_{16}H_{32}$ isomer
125	240	unknown
127	240	sat. hydrocarbon
128	240	$C_{15}H_{30}O$ isomer
128A	240	$C_{17}H_{34}$ isomer
129	240	*n*-heptadecane
130	240	sat. hydrocarbon
131	240	*n*-octadecane

Table C-8. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L4).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2A	53	C_4H_8 isomer
2B	53	*n*-butane
2C	54	acetaldehyde (tent.)
2D	54	C_4H_8 isomer
2E	56	C_5H_{10} isomer
3	58	isopentane
4	59	acetone
4A	59	C_5H_{10} isomer
5	60	*n*-pentane
5A	60	C_5H_{10} isomer
5B	61	isopropanol
5C	62	dichloromethane + C_5H_{10} isomer
6	63	methyl acetate
6A	64	C_5H_6 isomer
6B	64	CS_2
6C	66	2-methylpropanal
6D	67	C_5H_8 isomer
7	68	2-methylpentane
8	70	3-methylpentane
8A	71	C_6H_{12} isomer + methyl ethyl ketone (tent.)
9	72	hexafluorobenzene (es)
10	73	*n*-hexane
10A	73	isopropyl ether
11	74	chloroform + C_6H_{12} isomer
12	75	C_6H_{12} isomer
12A	75	ethyl acetate (tent.)
12B	76	C_6H_{12} isomer
13	76	perfluorotoluene (es)
14	77	C_6H_{12} isomer
14A	78	1,1,1-trichloroethane
15	80	1-chlorobutane
16	81	unknown
16A	82	C_6H_{10} isomer
17	82	benzene
17A	83	isopropyl acetate (tent.)
17B	83	carbon tetrachloride
17C	84	cyclohexane
18	84	2-methylhexane
18A	85	2,3-dimethylpentane
19	86	3-methylhexane
19A	87	C_6H_{10} isomer
19B	88	$C_5H_{10}O$ isomer
19C	88	C_7H_{14} isomer
20	88	dichloropropene
20A	89	C_7H_{16} isomer
21	89	trichloroethylene
21A	90	C_7H_{14} isomer
22	91	*n*-heptane
22A	92	C_7H_{14} isomer
22B	93	*n*-propyl acetate
23	94	C_7H_{14} isomer
23A	94	C_7H_{12} isomer
24	96	methylcyclohexane
24A	97	4-methyl-2-pentanone
24B	98	C_8H_{18} isomer
24C	98	dimethyl disulfide
25	98	C_8H_{18} isomer
26	100	C_8H_{16} isomer
27	102	C_8H_{18} + C_7H_{12} isomers (tent.)
28	104	toluene
29	105	C_8H_{18} isomer
30	107	C_8H_{18} isomer
31	108	C_8H_{16} isomer
32	109	C_8H_{18} isomer
32A	110	C_8H_{16} isomer
32B	110	1,2-dibromoethane (tent.)
33	111	C_8H_{16} isomer
34	112	*n*-octane
34A	113	C_8H_{16} isomer
35	114	tetrachloroethylene
35A	114	C_8H_{16} isomer
36	116	dimethylpentanal or $C_7H_{14}O$ isomer
37	117	C_9H_{20} isomer
37A	118	C_8H_{14} isomer (tent.)
38	118	C_9H_{20} isomer
39	119	4-vinylcyclohexene
39A	119	C_8H_{16} isomer
39B	120	C_9H_{18} isomer
40	120	C_9H_{20} isomer + ethylcyclohexane
41	121	trimethylcyclohexane isomer
41A	128	C_9H_{18} isomer
41B	123	C_9H_{16} isomer
41C	123	C_9H_{18} isomer
42	124	ethylbenzene
43	124	C_9H_{18} isomer
43A	125	C_9H_{20} isomer
44	125	xylene isomer
44A	126	C_9H_{20} isomer

(continued)

Table C-8. (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
45	127	C_9H_{20} isomer
46	128	$C_7H_{14}O$ + C_9H_{18} isomers
46A	129	C_9H_{18} isomer
47	129	styrene
47A	129	tetrahydroindene or C_9H_{12} isomer
48	130	*o*-xylene
48A	130	C_9H_{18} isomer
49	131	methylethylcyclohexane isomer
50	133	*n*-nonane
50A	134	anisole
50B	135	$C_{10}H_{20}$ isomer
50C	135	$C_{10}H_{22}$ isomer
51	136	C_3-alkyl cyclohexane isomer
51A	136	C_9H_{12} isomer
52	137	isopropylbenzene + $C_{10}H_{22}$ isomer
52A	138	$C_{10}H_{20}$ isomer
53	138	C_9H_{16} isomer
53A	139	$C_{10}H_{22}$ isomer
53B	140	$C_{10}H_{20}$ isomer
54	140	propylcyclohexane
54A	141	$C_{10}H_{22}$ isomer
55	141	$C_{10}H_{16}$ isomer
55A	142	$C_{10}H_{22}$ isomer
56	142	$C_{10}H_{20}$ isomer + benzaldehyde
57	143	*n*-propylbenzene
57A	143	$C_{10}H_{20}$ isomer
58	144	ethyltoluene isomer
58A	145	$C_{10}H_{22}$ isomer
59	145	1,3,5-trimethylbenzene + $C_{10}H_{22}$ isomer
59A	146	$C_{10}H_{20}$ isomer
60	147	$C_{10}H_{22}$ isomer
61	148	*o*-ethyltoluene
62	148	$C_{10}H_{18}$ isomer
63	149	$C_{10}H_{20}$ isomer
63A	150	C_3H_5-benzene isomer
64	150	1,2,4-trimethylbenzene
64A	151	$C_{10}H_{20}$ isomer
65	152	*n*-decane
65A	153	dichlorobenzene isomer (tent.)
66	153	$C_{10}H_{20}$ isomer
66A	154	C_4-alkyl benzene isomer
66B	154	$C_{11}H_{22}$ isomer (tent.)
67	155	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
68	156	1,2,3-trimethylbenzene
69	156	$C_{11}H_{24}$ isomer
70	157	$C_{11}H_{24}$ isomer + *o*-dichlorobenzene
70A	158	indan
71	159	C_4-alkyl cyclohexane isomer
71A	160	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
72	160	C_4-alkyl benzene isomer
73	161	C_4-alkyl benzene isomer + *n*-butylbenzene
74	162	$C_{11}H_{24}$ isomer
75	162	$C_{11}H_{22}$ isomer
75A	163	C_4-alkyl benzene isomer
76	163	$C_{11}H_{22}$ isomer
76A	163	C_4-alkyl benzene isomer
76B	164	$C_{10}H_{18}$ isomer
77	164	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
78	165	C_4-alkyl benzene isomer
78A	165	$C_{11}H_{20}$ isomer
78B	165	$C_{11}H_{22}$ isomer
79	166	C_4-alkyl benzene isomer
79A	166	$C_{12}H_{22}$ isomer
80	167	$C_{11}H_{22}$ isomer
81	168	$C_{11}H_{22}$ isomer
81A	168	$C_{12}H_{24}$ isomer
82	169	*n*-undecane
82A	170	C_4-alkyl benzene isomer
83	170	$C_{11}H_{22}$ isomer
83A	171	$C_{12}H_{24}$ isomer
83B	171	$C_{12}H_{26}$ isomer
83C	171	C_4-alkyl benzene isomer
84	172	$C_{12}H_{26}$ isomer
84A	173	$C_{11}H_{20}$ isomer
85	174	$C_{12}H_{26}$ isomer
85A	174	C_2-alkyl phenol isomer
86	175	C_5-alkyl benzene isomer
86A	175	$C_{12}H_{24}$ isomer
86B	176	C_5-alkyl benzene + C_4H_7-benzene isomers
87	177	C_5-alkyl cyclohexane isomer
87A	177	$C_{11}H_{20}$ isomer

(continued)

Table C-8. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
87B	177	C_5-alkyl benzene + C_2-alkyl phenol isomer
87C	178	C_4H_7-benzene + $C_{12}H_{24}$ isomers
88	178	$C_{12}H_{26}$ + tetramethylbenzene isomers
89	179	C_5-alkyl benzene isomer
90	180	1,2,3,4-tetrahydronaphthalene + C_5-alkyl benzene isomer
90A	180	C_6-alkyl benzene isomer
91	181	C_5-alkyl benzene + $C_{12}H_{26}$ isomers
91A	182	$C_{12}H_{24}$ isomer
92	183	naphthalene
92A	184	$C_{12}H_{24}$ isomer
92B	184	C_5-alkyl benzene isomer
93	185	*n*-dodecane
94	186	C_5-alkyl benzene isomer
95	187	$C_{13}H_{28}$ isomer
96	188	C_6-alkyl benzene isomer
96A	190	C_6-alkyl benzene isomer
97	191	$C_{13}H_{26}$ isomer
98	192	C_6-alkyl cyclohexane isomer
98A	192	$C_{13}H_{26}$ isomer
99	193	$C_{13}H_{28}$ isomer
100	194	C_6-alkyl benzene isomer
100A	195	$C_{13}H_{28}$ isomer
101	196	$C_{14}H_{30}$ isomer
101A	197	$C_{11}H_{22}O$ isomer
102	198	$C_{13}H_{26}$ isomer
103	199	*n*-tridecane
103A	200	β-methylnaphthalene
104	201	C_5-alkyl benzene + $C_{13}H_{26}$ isomers
105	202	α-methylnaphthalene
105A	203	C_6H_{11}-benzene isomer (tent.)
105B	205	C_7-alkyl benzene isomer
105C	206	$C_{14}H_{28}$ isomer
106	207	C_7-alkyl cyclohexane or $C_{13}H_{26}$ isomer
106A	208	$C_{15}H_{32}$ isomer
107	209	$C_{10}H_{10}O$ ketone isomer
107A	210	$C_{15}H_{30}$ isomer
108	211	biphenyl
108A	211	$C_{14}H_{28}$ isomer
109	213	*n*-tetradecane + diphenyl ether
110	215	dimethylnaphthalene isomer
111	217	dimethylnaphthalene isomer
111A	218	$C_{15}H_{30}$ isomer
112	220	$C_{15}H_{32}$ isomer
113	222	$C_{16}H_{34}$ isomer
113A	224	$C_{15}H_{30}$ isomer
113B	225	$C_{15}H_{30}$ isomer
114	226	*n*-pentadecane
115	228	unknown
115A	231	$C_{15}H_{30}$ isomer
115B	232	C_3-alkyl naphthalene isomer
116	235	diethyl phthalate
117	237	$C_{14}H_{28}O$ isomer
117A	237	$C_{16}H_{32}$ isomer
118A	239	*n*-hexadecane
119	240	unknown
119A	240	benzophenone
120	240	$C_{17}H_{34}$ isomer
120A	240	$C_{17}H_{36}$ isomer
121	240	sat. hydrocarbon
122	240	$C_{15}H_{30}O$ isomer
123	240	*n*-heptadecane
124	240	$C_{19}H_{40}$ isomer

Table C-9. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L5).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
4	52	n-propane (tent.)
4A	53	butene
5	53	n-butane
6	55	acetaldehyde
7	58	isopentane
7A	58	dimethyl ether
8	59	acetone
8A	61	dichloroethylene isomer
9	62	dichloromethane
10A	65	C_4H_8O isomer
10B	68	C_6H_{12} isomer (tent.)
11	68	2-methylpentane
12	70	3-methylpentane
13	72	hexafluorobenzene (es)
14	73	n-hexane
14A	73	diisopropyl ether
15	74	chloroform
15A	75	ethyl acetate (tent.)
16	77	perfluorotoluene (es)
16A	78	methylcyclopentane
17	83	benzene
17A	84	carbon tetrachloride
17B	94	cyclohexane
17C	95	2-methylhexane
18	87	C_7H_{16} isomer
18A	89	C_7H_{14} isomer (tent.)
19	90	acetic acid
20	92	n-heptane
20A	93	C_7H_{14} + $C_5H_{10}O$ isomers (tent.)
20B	97	methylcyclohexane
20C	99	C_7H_{10} isomer (tent.)
20D	102	C_8H_{16} isomer
20E	102	C_8H_{18} isomer
21	104	toluene
21A	105	C_8H_{18} isomer
21B	107	C_8H_{18} isomer
22	110	n-hexanal
23	113	n-octane
23A	115	tetrachloroethylene (tent.)
23B	124	ethylbenzene
24	126	xylene isomer
24A	129	C_9H_{20} isomer
24B	130	styrene
24C	131	n-heptanal
25	131	o-xylene + C_9H_{20} isomer
26	133	n-nonane
27	137	$C_{10}H_{22}$ isomer
27A	140	$C_{10}H_{22}$ isomer
27B	141	$C_{10}H_{16}$ isomer
27C	142	$C_8H_{16}O$ isomer
28	143	benzaldehyde
28A	143	n-propylbenzene
28B	144	ethyltoluene isomer
29	146	$C_{11}H_{24}$ isomer
29A	147	phenol
29B	148	C_3-alkyl benzene isomer
30	149	$C_{11}H_{24}$ isomer
31	150	n-octanal
31A	150	$C_{10}H_{20}$ isomer
31B	151	1,2,4-trimethylbenzene
32	152	n-decane
32A	155	1,2,3-trimethylbenzene + $C_{11}H_{24}$ isomer
33	157	$C_{11}H_{24}$ isomer
33A	159	unsat. hydrocarbon
34	160	sat. hydrocarbon
34A	161	C_4-alkyl benzene isomer
35	162	acetophenone
35A	163	cresol isomer
35B	164	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
35C	165	C_4-alkyl benzene isomer
35D	166	$C_{11}H_{22}$ isomer
35E	166	C_4-alkyl benzene isomer
36	167	n-nonanal
36A	168	$C_{11}H_{22}$ isomer
37	169	n-undecane
37A	172	C_4-alkyl benzene isomer
37B	174	$C_{12}H_{24}$ isomer
38	175	dimethylphenol isomer
38A	176	$C_{12}H_{24}$ isomer
38B	177	$C_{12}H_{26}$ isomer
39	178	C_2-alkyl phenol isomer
39A	180	C_4-alkyl benzene + $C_{12}H_{24}$ isomers
39B	182	C_3-alkyl phenol isomer
40	184	n-decanal + naphthalene
40A	185	$C_{12}H_{24}$ isomer
41	186	n-dodecane
41A	187	C_3-alkyl phenol isomer
41B	188	$C_{12}H_{24}$ isomer

(continued)

Table C-9. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
41C	193	$C_{12}H_{24}$ isomer
41D	197	$C_{11}H_{20}O$ isomer (tent.)
41E	198	$C_{13}H_{26}$ isomer
42	199	n-undecanal
43	200	n-tridecane
43A	201	β-methylnaphthalene
43B	205	$C_{14}H_{30}$ isomer
44	207	alkyl butyrate
44A	208	biphenyl (tent.)
44B	209	$C_{14}H_{28}$ isomer
45	210	n-tetradecane
47	222	sat. hydrocarbon
47A	223	$C_{15}H_{30}$ isomer

Table C-10. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 3, P1/L8).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2	7	60	n-pentane
3	51	acetaldehyde	7A	60	dichloroethylene isomer
3A	52	C_4H_8 isomer	7B	61	methylene chloride
4	53	isobutane	7C	61	C_5H_{10} isomer
4A	54	C_4H_8	9	67	2-methylpentane
4B	55	C_4H_8	10	69	3-methylpentane
5	56	n-butane	11	70	hexafluorobenzene (eI)
5A	56	C_5H_{10}	12	71	n-hexane
6	57	isopentane	13	75	perfluorotoluene (eI)
6A	59	acetone	14	76	methylcyclopentane

Table C-11. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 3, P1/L8).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
3	53	propane
3A	55	C_4H_{10} isomer
3B	56	acetaldehyde
3C	56	butane
4	58	isopentane
5	59	methyl acetate (tent)
5A	60	dimethyl ether
5B	60	acetone
6	62	*n*-pentane
6A	63	$C_4H_{10}O$ isomer (tent)
7	63	methylene chloride
7A	69	C_6H_{12} isomer
7B	69	C_5H_{10} isomer
10	70	2-methylpentane
10A	71	C_6H_{12} isomer
11	73	3-methylpentane
11A	73	butanal (tent)
11B	73	C_6H_{12} isomer
12	75	hexafluorobenzene (e■)
12A	75	*n*-hexane
13	76	isopropyl ether
13A	76	chloroform
13B	78	methyl ethyl ketone (tent)
14	80	perfluorotoluene (e■)
14A	81	C_6H_{12} isomer (tent)
15	83	1,1,1-trichloroethane
16	86	benzene
16A	87	carbon tetrachloride
16B	87	cyclohexane
17	88	2-methylhexane
17A	89	2,3-dimethylpentane
18	90	3-methylhexane
19	92	C_7H_{14} isomer
19A	93	$C_5H_{10}O$ isomer
20	95	*n*-heptane
20A	97	$C_6H_{12}O$ isomer (tent)
20B	100	methylcyclohexane
21	101	4-methyl-2-pentanone
22	104	$C_6H_{10}O$ ketone isomers (tent)
22A	106	2-hexanol
23	108	toluene
24	110	C_8H_{18} isomer
25	113	4-methyl-3-penten-2-one
26	115	*n*-octane
27	117	tetrachloroethylene
27A	118	C_8H_{16} isomer
28	119	2-methoxy-2h-dihydro-pyran
28A	122	C_9H_{20} isomer
29	123	C_8H_{16} isomer
29A	124	chlorobenzene + ethylcyclohexane
29B	125	C_9H_{18} isomer
30	127	ethylbenzene
31	129	xylene isomer
31A	129	C_9H_{20} isomer
32	130	C_9H_{20} isomer
32A	130	heptanone isomer
33	132	styrene
34	133	*o*-xylene
34A	134	C_9H_{18} isomer
35	135	*n*-nonane
36	138	C_9H_{18} isomer
37	139	isopropylbenzene + $C_{10}H_{22}$ isomer
37A	140	$C_{10}H_{22}$ isomer
38	142	$C_{10}H_{22}$ + C_3-alkyl cyclohexane isomers
38A	143	$C_{10}H_{16}$ isomer
39	143	benzadehyde
40	144	*n*-propylbenzene
40A	145	ethyltoluene isomer
41	146	$C_9H_{18}O$ ketone isomer
41A	147	phenol
41B	147	cyanobenzene + 1,3,5-trimethylbenzene
42	147	$C_{10}H_{22}$ isomer
42A	148	$C_{10}H_{20}$ isomer
42B	148	$C_{10}H_{22}$ isomer
42C	149	*o*-ethyltoluene
43	149	$C_9H_{18}O$ ketone isomer
43A	150	$C_{10}H_{22}$ isomer
43B	151	benzofuran + $C_{10}H_{20}$ isomer
44	152	1,2,4-trimethylbenzene
45	153	*n*-decane
46	154	dichlorobenzene isomer
46A	155	$C_{10}H_{20}$ isomer
46B	155	C_4-alkyl benzene isomer
46C	156	$C_{11}H_{24}$ + C_4-alkyl benzene
-	-	isomers
46D	157	$C_{10}H_{20}$ isomer
47	157	1,2,3-trimethylbenzene

(continued)

Table C-11. (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
47A	157	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
48	159	o-dichlorobenzene
48A	159	C_4-alkyl cyclohexane isomer + indan
48B	160	$C_{11}H_{24}$ isomers
48C	161	indene + $C_{11}H_{22}$ isomers
48D	161	C_3-alkyl pyridine isomer (tent)
48E	161	C_4-alkyl benzene isomer
48F	162	C_4-alkyl benzene isomer
49	162	acetophenone
49A	163	C_4-alkyl benzene isomer
50	165	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
51	166	$C_{11}H_{24}$ isomer
51A	166	C_4-alkyl benzene isomer
51B	167	C_4H_7-benzene isomer
52	168	C_4-alkyl benzene isomer
52A	168	$C_{11}H_{22}$ isomer
53	169	n-nonanal
53A	169	C_4H_7-benzene isomer
53B	170	$C_{11}H_{22}$ isomer
54	171	n-undecane
54A	172	C_4-alkyl benzene isomer
55	173	3,5,5-trimethyl-2-cyclohexenone
55A	174	C_4alkyl benzene isomer
55B	175	2-pyrone (tent)
55C	175	$C_{11}H_{20}$ isomer
55D	175	$C_{11}H_{22}$ isomer
55E	176	C_5-alkyl benzene isomer
55F	178	C_4H_7-benzene isomer
55G	178	unsat. hydrocarbon
56	180	$C_{12}H_{26}$ isomer
56A	180	C_5-alkyl benzene isomer
57	181	1,2,3,4-tetrahydronaphthalene
57A	183	C_5-alkyl benzene isomer
58	185	naphthalene
58A	186	2,3-benzothiophene (tent)
59	187	n-dodecane
60	188	2,6,8-trimethylnonanone-4
60A	192	methyldihydronaphthalene isomer (tent.)
60B	196	$C_{12}H_{24}O$ isomer (tent)
60C	198	$C_{13}H_{28}$ isomer
60D	200	unsat. hydrocarbon
61	202	n-tridecane
61A	203	β-methylnaphthalene
61B	205	α-methylnaphthalene
61C	209	$C_{15}H_{32}$ isomer (tent)
62	213	α-tetralone
63	214	biphenyl
64	216	diphenyl ether + n-tetradecane
64A	217	$C_{14}H_{28}$ isomer
64B	218	C_2-alkyl naphthalene isomer
64C	220	C_2-alkyl naphthalene isomer
64D	228	$C_{15}H_{30}$ isomer
65	229	n-pentadecane
65A	231	$C_{14}H_{12}$ isomer
68	240	benzophenone
68A	240	$C_{17}H_{36}$ isomer

Table C-12. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L1).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
3	51	propane (tent)
4	52	C_4H_{10} isomer (tent)
5	53	acetaldehyde
6	56	*n*-butane
7	58	isopentane
9	60	acetone
9A	61	diethyl ether
10	61	*n*-pentane
10A	61	Background peak
11	62	methylene chloride
13	65	C_6H_{14} isomer (tent)
14A	68	C_5H_{10} isomer
15	69	2-methylpentane
16	71	3-methylpentane
16A	72	C_6H_{12} isomer
17	73	hexafluorobenzene (es)
18	74	*n*-hexane
19	75	chloroform
20	76	ethyl acetate
20A	77	C_6H_{12} isomer
21	78	perfluorotoluene (es)
22	79	methylcyclopentane
23	80	unsat. hydrocarbon (tent)
24	81	1,1,1-trichloroethane
24A	82	C_7H_{14} isomer
24B	83	C_6H_{10} isomer
25	84	benzene
26	85	carbon tetrachloride
26A	86	cyclohexane
27	86	2-methylhexane
27A	87	2,3-dimethylpentane
28	87	acetic acid
29	88	3-methylhexane
30	90	C_7H_{14} isomer
30A	91	C_7H_{14} isomer
31	91	C_8H_{18} isomer
31A	92	C_7H_{14} isomer
32	93	*n*-heptane
33	94	C_7H_{14} isomer
34	99	methylcyclohexane
34A	100	C_8H_{16} isomer
35	101	C_8H_{18} isomer
35A	102	$C_6H_{12}O$ isomer
36	103	C_8H_{16} isomer
36A	104	C_8H_{16} isomer
37	105	C_8H_{18} isomer
38	106	toluene
39	108	C_8H_{18} isomer
40	109	C_8H_{18} isomer
40A	111	C_8H_{16} isomer
41	112	C_9H_{20} isomer
41A	113	C_8H_{16} isomer
42	115	*n*-octane
43	116	tetrachloroethylene
43A	117	C_8H_{16} isomer
43B	119	C_9H_{20} isomer
43C	120	C_9H_{20} isomer
43D	121	C_9H_{20} isomer
43E	122	C_8H_{16} isomer
44	123	ethylcyclohexane + C_9H_{20} isomers
44A	124	C_9H_{18} isomer
44B	125	C_9H_{18} isomer
45	127	ethylbenzene
45A	127	C_9H_{18} isomer
46	128	xylene isomer
46A	129	C_9H_{20} isomer
47	130	C_9H_{20} isomer
47A	132	C_9H_{20} isomer
48	132	styrene
49	133	*o*-xylene
49A	134	$C_{10}H_{22}$ isomer
49B	134	C_9H_{18} isomer
50	136	*n*-nonane
50A	138	C_9H_{18} isomer
51	139	$C_{10}H_{22}$ isomer + isopropylbenzene
51A	140	$C_{10}H_{20}$ isomer
52	141	$C_{10}H_{22}$ isomer
53	143	$C_{10}H_{22}$ isomer
53A	143	$C_{10}H_{20}$ isomer
54	144	$C_{10}H_{16}$ isomer
55	144	benzaldehyde
56	145	*n*-propylbenzene
57	146	ethyltoluene isomer
57A	147	$C_{10}H_{22}$ isomer
57B	148	phenol
57C	148	1,3,5-trimethylbenzene
58	148	$C_{11}H_{24}$ isomer
58A	150	$C_{10}H_{22}$ isomer
58B	150	*o*-ethyltoluene

continued

Table C-12. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
58C	151	$C_{10}H_{22}$ isomer
58D	152	$C_{10}H_{16}$ isomer
58E	152	C_3H_5-benzene + $C_{10}H_{20}$ isomers
59	153	1,2,4-trimethylbenzene
59A	154	$C_{10}H_{20}$ isomer
60	155	*n*-decane
61	156	dichlorobenzene isomer
61A	156	$C_{10}H_{20}$ isomer
61B	157	C_4-alkyl benzene isomer
61C	158	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
62	158	1,2,3-trimethylbenzene
62A	159	$C_{11}H_{24}$ isomer
63	160	$C_{12}H_{26}$ isomer
63A	161	indan
63B	162	C_4-alkyl cyclohexane isomer
63C	162	$C_{11}H_{22}$ isomer
63D	163	C_4-alkyl benzene isomer
64	163	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
65	164	acetophenone
65A	164	C_4-alkyl benzene isomer
65B	165	$C_{11}H_{24}$ isomer
65C	165	$C_{11}H_{22}$ isomer
66	166	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
66A	168	$C_{11}H_{24}$ isomer
66B	168	C_4-alkyl benzene isomer
66C	169	$C_{12}H_{24}$ isomer
66D	169	C_4H_7-benzene isomer
67	169	C_4-alkyl benzene isomer
67A	170	$C_{12}H_{26}$ isomer
68	170	*n*-nonanal
68A	171	$C_{11}H_{22}$ isomer
69	172	*n*-undecane
69A	173	C_5-alkyl benzene isomer
69B	173	C_4-alkyl benzene isomer
69C	174	$C_{11}H_{22}$ isomer
70	176	C_4-alkyl benzene isomer
70A	177	$C_{12}H_{26}$ isomer
70B	178	C_2-alkyl phenol isomer
70C	178	C_5-alkyl benzene isomer
70D	179	C_5-alkyl benzene isomer
70E	180	C_5-alkyl cyclohexane isomer
70F	180	$C_{12}H_{24}$ + C_5-alkyl benzene isomers
70G	181	C_4H_7-benzene isomer
71	182	$C_{12}H_{26}$ + C_5-alkyl benzene isomers
71A	182	$C_{12}H_{24}$ isomer
71B	183	C_4-alkyl benzene isomer
71C	183	C_5-alkyl benzene isomer
71D	184	$C_{12}H_{26}$ isomer
71E	184	C_5-alkyl benzene isomer
71F	185	$C_{10}H_{20}O$ isomer
71G	186	naphthalene
72	187	*n*-decanal
72A	187	$C_{12}H_{24}$ isomer
72B	188	C_5-alkyl benzene isomer
73	189	*n*-dodecane
73A	190	C_5-alkyl benzene isomer
73B	190	$C_{12}H_{24}$ isomer
73C	196	$C_{13}H_{28}$ isomer
73D	200	$C_{13}H_{28}$ isomer
73E	202	$C_{12}H_{24}$ isomer
74	204	*n*-tridecane
74A	204	β-methylnaphthalene
74B	205	$C_{13}H_{26}$ isomer
74C	206	α-methylnaphthalene
75	211	C_5-alkyl cyclohexane isomer
75A	216	$C_{14}H_{28}$ isomer
76	218	*n*-tetradecane
76A	220	dimethylnaphthalene isomer
76B	222	dimethylnaphthalene isomer
76C	224	$C_{15}H_{30}$ isomer
76D	230	$C_{15}H_{30}$ isomer
77	231	*n*-pentadecane
78	235	unknown
79A	240	$C_{16}H_{32}$ isomer
80A	240	*n*-hexadecane
80B	240	benzophenone

Table C-13. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L2).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
3A	52	propane (tent)
3B	52	C_4H_8 isomer
4	53	C_4H_{10} isomer
4A	54	acetaldehyde
4B	59	isopentane
4C	61	C_5H_{10} isomer
4D	61	furan (tent)
5	62	acetone + *n*-pentane
5A	63	diethyl ether (tent)
5B	64	dichloroethylene isomer (traces)
6	64	methylene chloride
7A	71	C_5H_{10} isomer
8	71	2-methylpentane
8A	73	$C_5H_{10}O$ isomer
9	74	3-methylpentane
9A	74	butanal
9B	75	C_6H_{12} isomer
10	76	hexafluorobenzene (eI)
11	77	*n*-hexane
12	77	chloroform
12A	80	C_6H_{12} isomer
13	81	perfluorotoluene (eI)
14	82	methylcyclopentane
14A	84	1,1,1-trichloroethane
14B	86	C_6H_{10} isomer (tent)
15	87	benzene
15A	88	carbon tetrachloride (traces)
15B	88	cyclohexane
16	89	2-methylhexane
16A	90	2,3-dimethylpentane (tent)
17	91	3-methylhexane + acetic acid
18	93	C_7H_{14} isomer
18A	94	trichloroethylene
18B	94	C_8H_{18} isomer
19	96	*n*-heptane
19A	98	C_7H_{14} isomer
20	101	methylcyclohexane
21	103	C_8H_{18} isomer
21A	103	$C_6H_{12}O$ ketone isomer
21B	105	C_8H_{16} isomer
21C	106	C_8H_{16} isomer
22	107	C_8H_{18} isomer
23	108	toluene
24	109	C_8H_{18} isomer
25	111	C_8H_{18} isomer
25A	112	$C_6H_{12}O$ isomer
25B	112	C_8H_{16} isomer
26	113	*n*-hexanal + C_9H_{20} isomer
26A	114	C_8H_{16} isomer
27	116	*n*-octane
28	117	tetrachloroethylene
28A	118	C_8H_{16} isomer
28B	119	C_9H_{20} isomer (tent)
29	119	C_9H_{20} isomer
29A	121	C_9H_{20} isomer
29B	121	C_8H_{16} isomer
30	122	C_9H_{20} isomer
30A	123	C_9H_{18} isomer
31	124	C_9H_{20} isomer + ethylcyclohexane
31A	125	C_9H_{18} isomer
31B	126	$C_7H_{14}O$ isomer (tent)
32	127	ethylbenzene isomer
32A	128	C_9H_{18} isomer
33	129	xylene isomer
33A	129	C_9H_{20} isomer
34	130	C_9H_{20} isomer
34A	131	$C_7H_{14}O$ isomer
35	132	$C_{10}H_{22}$ isomer
35A	132	styrene
35B	133	C_9H_{18} isomer
36	133	*o*-xylene
36A	134	C_9H_{18} isomer
37	136	*n*-nonane
38	138	C_9H_{18} isomer
39	139	$C_{10}H_{22}$ isomer + isopropylbenzene
39A	140	$C_{10}H_{20}$ isomer
40	141	$C_{10}H_{22}$ isomer
40A	141	C_9H_{16} isomer (tent)
40B	142	$C_{10}H_{22}$ isomer
41	142	$C_{10}H_{22}$ isomer
41A	143	C_3-alkyl cyclohexane isomer
42	144	benzaldehyde
42A	145	$C_{10}H_{20}$ isomer
43	145	*n*-propylbenzene
44	146	ethyltoluene isomer
44A	147	$C_{10}H_{22}$ isomer
45	148	1,3,5-trimethylbenzene
45A	148	$C_{11}H_{24}$ isomer

(continued)

Table C-13. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
45B	149	phenol (tent) + $C_{10}H_{20}$ isomer
46	149	$C_{10}H_{22}$ isomer
47	150	*o*-ethyltoluene
47A	151	$C_{10}H_{22}$ isomer
47B	151	$C_{11}H_{24}$ isomer
48	152	*n*-octanal
49	153	1,2,4-trimethylbenzene
49A	153	$C_{10}H_{20}$ isomer
50	154	*n*-decane
51	155	dichlorobenzene isomer
51A	155	isobutylbenzene
51B	156	sec-butylbenzene
52	157	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
53	158	1,2,3-trimethylbenzene
53A	158	$C_{11}H_{24}$ isomer
54	159	$C_{11}H_{24}$ isomer
55	160	C_3H_5-benzene isomer
55A	161	$C_{11}H_{24}$ isomer
55B	161	C_4-alkyl cyclohexane isomer
55C	161	$C_{11}H_{22}$ isomer
55D	162	C_4-alkyl benzene isomer
56	162	p-propyltoluene
57	163	C_4-alkyl benzene isomer + acetophenone (tent.)
57A	164	C_4-alkyl benzene isomer
57B	164	$C_{11}H_{24}$ isomer
58	166	*o*-propyltoluene
58A	167	$C_{11}H_{24}$ isomer
59	167	C_4-alkyl benzene isomer
59A	168	$C_{11}H_{24}$ isomer
60	169	C_4-alkyl benzene isomer
60A	169	*n*-nonanal + C_4H_7-benzene isomer
61	170	C_4-alkyl benzene isomer
61A	170	$C_{11}H_{22}$ isomer
62	171	*n*-undecane + C_5-alkyl benzene . isomer
63	172	C_4-alkyl benzene isomer
63A	173	$C_{11}H_{22}$ isomer
63B	173	C_5-alkyl benzene isomer
63C	173	$C_{12}H_{24}$ isomer
63D	174	$C_{12}H_{26}$ isomer
64	174	tetramethylbenzene isomer
65	175	C_4-alkyl benzene isomer
65A	176	$C_{12}H_{26}$ isomer
66	177	C_5-alkyl benzene isomer
66A	178	C_4H_7-benzene isomer
67	178	C_5-alkyl benzene isomer
67A	178	C_4H_7-benzene isomer
67B	179	$C_{12}H_{24}$ isomer
68	179	C_5-alkyl benzene isomer
69	180	C_4H_7-benzene isomer
70	181	C_4-alkyl benzene isomer
70A	181	C_5-alkyl benzene isomer
70B	182	C_5-alkyl benzene isomer
71	182	1,2,3,4-tetrahydronaphthalene
71A	182	C_5-alkyl benzene isomer
72	183	C_5-alkyl benzene isomer
72A	184	C_4-alkyl benzene isomer
72B	185	C_6-alkyl benzene isomer
72C	185	C_5H_9-benzene + C_5-alkyl benzene isomers
73	186	naphthalene
73A	186	C_5H_9-benzene isomer
73B	186	C_5-alkyl benzene isomer
74	187	C_5-alkyl benzene isomer + *n*-dodecane
74A	188	C_6-alkyl benzene isomer
75	189	C_5-alkyl benzene isomer
75A	190	$C_{13}H_{28}$ isomer
76	191	C_6-alkyl benzene isomer
76A	192	C_5-alkyl benzene isomer
76B	193	C_5-alkyl benzene isomer
77	194	$C_{13}H_{26}$ isomer
77A	195	C_6-alkyl benzene isomer
77B	195	C_5-alkyl benzene isomer
77C	195	$C_{13}H_{28}$ isomer
77D	196	C_5H_9-benzene isomer
77E	196	C_6-alkyl benzene isomer
77F	196	C_5-alkyl benzene isomer
77G	197	$C_{13}H_{28}$ isomer
77H	197	C_5-alkyl benzene isomer
78	199	$C_{14}H_{30}$ isomer
78A	200	$C_{13}H_{26}$ isomer
78B	200	C_5-alkyl benzene isomer
78C	201	$C_{13}H_{26}$ isomer
79	202	*n*-tridecane
79A	203	β-methylnaphthalene
80	204	C_5-alkyl benzene isomer
80A	205	C_6-alkyl benzene isomer
81	205	α-methylnaphthalene

(continued)

Table C-13. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
81A	209	C_5H_9-benzene + C_6-alkyl benzene isomers
82	210	C_6-alkyl benzene isomer
83	213	1,2,3,4-tetrahydronaphthalen-1-one
83A	214	biphenyl
83B	214	$C_{14}H_{30}$ isomer
83C	215	$C_{14}H_{28}$ isomer
84	216	n-tetradecane
84A	218	$C_{10}H_{10}O$ isomer (tent)
84B	219	dimethylnaphthalene isomer
84C	220	dimethylnaphthalene isomer
84D	223	$C_{15}H_{30}$ isomer
84E	225	$C_{15}H_{32}$ isomers
84F	227	$C_{13}H_{26}O$ isomer
84G	228	$C_{15}H_{30}$ isomer
85	229	n-pentadecane
86	233	unknown
88A	240	n-hexadecane
88B	240	benzophenone
88C	240	$C_{17}H_{36}$ isomer
88D	240	alkyl ketone
88E	240	n-heptadecane

Table C-14. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L9).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	47	CO_2
3	51	propane
4	53	isobutane
4A	54	C_4H_2 isomer
5	56	n-butane
6	58	isopentane
7	59	acetone
8	60	n-pentane
8A	61	diethyl ether
8B	62	vinylidine chloride
9	62	methylene chloride
11	64	CS_2
12	69	2-methylpentane
13	71	3-methylpentane
13A	72	C_5H_{12} isomer
14	73	hexafluorobenzene (eS)
15	74	n-hexane
15A	75	chloroform
16	76	C_7H_{16} isomer (tent.)
17	78	perfluorotoluene (eS)
18	79	methylcyclopentane

APPENDIX D

SEMIVOLATILE COMPOUNDS IDENTIFIED IN AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV

Table D-1. COMPOUNDS IDENTIFID IN POLAR NEUTRAL FRACTION OF <1.7 μ AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(Trip 3, P1/L1)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	124	naphthalene	18	259	a phthalate
2	135	benzothiazole (tent.)	19	263	a phthalate
3	161	Si compound (bkg.)	20	265	$C_{18}H_{10}$ isomer[4] (tent.)
4	167	C_4 alkyl benzene	21	265	$C_{18}H_{14}$ isomer[5]
5	168	naphthol + unknown	22	265	$C_{18}H_{10}$ isomer[4] (tent.)
6	182	unknown	23	265	$C_{18}H_{12}$ isomer[6]
7	196	p-nonyl phenol	24	265	benzanthrone
8	202	$C_{14}H_{10}$ isomer	25	265	a phthalate (bkg.)
9	212	a phthalate (bkg.)	26	265	methylbenzanthracene isomer or
10	213	$C_{13}H_9N$ isomer[1] (tent.)			methylbenzophenanthrene isomer[7]
11	216	$C_{13}H_8O$ isomer[2] (tent.)	27		triphenylphospine sulfide
12	217	C_2 alkyl fluorene (tent.)			(bkg.)
13	221	methyl hexadecanoate	28	265	unknown
14	222	a phthalate (bkg.)	29	265	$C_{20}H_{12}$ isomer[8]
15	234	$C_{16}H_{10}$ isomer[3]	30	265	$C_{20}H_{12}$ isomer[8] (tent.)
16	239	$C_{16}H_{10}$ isomer[3]	31	265	$C_{20}H_{12}$ isomer[8]
17	243	methyl octadecanoate +	32	265	binaphthyl isomer + unknown
		unknown(s)	33	265	unknown

1. $C_{13}H_9H$ isomers include benzoquinoline isomers and acridine.
2. $C_{13}H_8O$ isomers include fluorenones and perinaphthindenones and benzoindenones.
3. $C_{16}H_{10}$ isomers include pyrene and fluoranthene.
4. $C_{18}H_{10}$ isomers include 1,10-benzfluoranthene, 3,4-cyclopentapyrene and 1,10-benzoaceanthrylene.
5. $C_{18}H_{14}$ isomers include terphenyl isomers.
6. $C_{18}H_{12}$ isomers include benzanthracene isomers (naphthacene et al.) and benzophenanthrene isomers (triphenylene, chrysene et al.)
7. This compound is not a methylchrysene or a methyltriphenylene.
8. $C_{20}H_{12}$ isomers include perylene, benzpyrene isomers, and benzfluoranthene isomers.

Table D-2. COMPOUNDS IDENTIFIED IN PNA FRACTION OF <1.7 μ AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV (Trip 3, P1/L1)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	111	unknown + dichloromethane (solvent)
2	116	Si compound (bkg.)
3	122	unknown
4	123	naphthalene
5	124	Si compound (bkg.)
6	125	unknown
7	132	unknown
8	143	unknown
9	144	methylnaphthalene isomer (tent.)
10	151	$C_{12}H_{10}$ isomer
11	155	unknown
12	156	dimethylnaphthalene isomer + unknown
13	159	biphenylene (tent.)
14	160	unknown
15	162	di-t-butylbenzoquinone (bkg.?)
16	168	dibenzofuran (tent.)
17	169.5	unknown
18	173	trimethylnaphthalene isomer (tent.) + a phthalate (bkg.)
19	175	C_3 alkyl naphthalene (tent.)
20	177	fluorene
21	181	2,2,4-trimethylpenta-1,3-diol di-isobutyrate (bkg.)
22	184	hydroxyfluorene (tent.)
23	191	C_4 alkyl naphthalene (tent.)
24	193	methylfluorene isomer (tent.)
25	195	unknown
26	201	$C_{14}H_{10}$ isomer[2]
27	208	dimethylfluorene + unknown
28	211	methyldibenzothiophene isomer (tent.)
29	212	a phthalate (bkg.)
30	216	methyl $C_{14}H_{10}$ isomer[2]
31	217	4,5-methylenephenanthrene
32	219	methyl $C_{14}H_{10}$ isomer[2]
33	211	unknown(s)
34	222	a phthalate (bkg.)
35	229	dimethylphenanthrene isomer
36	230	diphenyloxazole isomer(s) (tent.)
37	231	dimethylphenanthrene isomer
38	233	$C_{16}H_{10}$ isomer[3]
39	236	$C_{16}H_{10}$ isomer[3]
40	239	$C_{16}H_{10}$ isomer[3]
41	243	trimethylphenanthrene isomer
42	244	trimethylphenanthrene isomer
43	246	trimethylphenanthrene isomer
44	247	benzofluorene isomer
45	249	$C_{17}H_{12}$ isomer[4]
46	251	methylpyrene isomer (tent.)
47	252	methylpyrene isomer (tent.)
48	255	methylpyrene isomer
49	261	C_4 alkyl $C_{14}H_{10}$ isomer (tent.)
50	264	a phthalate
51	265	terphenyl isomer (tent.)
52	265	terphenyl isomer (tent.)
53	265	$C_{18}H_{10}$ isomer[5]
54	265	terphenyl isomer
55	265	$C_{18}H_{10}$ isomer[5]
56	265	$C_{18}H_{12}$ isomer[6]
57	265	a phthalate (bkg.)
58	265	unknown
59	265	unknown
60	265	$C_{19}H_{14}$ isomer[7] (tent.)
61	265	phthalate(s) (bkg.)
62	265	phthalate(s) (bkg.)
63	265	$C_{19}H_{14}$ isomer[7] (tent.)
64	265	methyl $C_{18}H_{10}$ isomer[5] (tent.) + C_2 alkyl terphenyl (tent.)
65	265	C_2 alkyl $C_{18}H_{12}$ isomer[6]
66	265	C_2 alkyl $C_{18}H_{12}$ isomer[6]
67	265	C_2 alkyl $C_{18}H_{12}$ isomer[6]
68	265	$C_{22}H_{12}$ isomer[8] (tent.)
69	265	$C_{20}H_{12}$ isomer[9]
70	265	$C_{22}H_{12}$ isomer[8] (tent.)
71	265	$C_{21}H_{20}$ isomer[10] (tent.)
72	265	$C_{20}H_{12}$ isomer[9] (tent.)
73	265	C_2 alkyl $C_{18}H_{12}$ isomer[6] (tent.)
74	265	$C_{22}H_{12}$ isomer(s)[8] (tent.)
75	265	$C_{21}H_{16}$ isomer[11] (tent.)
76	265	$C_{21}H_{17}$ isomer[11] (tent.)
77	265	$C_{22}H_{12}$ isomer[8] (tent.)
78	265	$C_{20}H_{14}$ isomer[12] (tent.)
79	265	$C_{20}H_{12}$ isomer[9] (tent.)
80	265	$C_{22}H_{12}$ isomer[8] (tent.)
81	265	$C_{21}H_{16}$ isomer[11] (tent.)
82	265	$C_{21}H_{18}$ isomer[13] (tent.)
83	265	$C_{23}H_{14}$ isomer[14] (tent.)
84	265	$C_{20}H_{12}$ isomer[9] (tent.)
85	265	$C_{21}H_{16}$ isomer[11] (tent.)

(continued)

Table D-2. (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
86	265	$C_{21}H_{14}$ isomer(s)[15] (tent.)
87	265	$C_{21}H_{18}$ isomer[13] (tent.)
88	265	$C_{21}H_{14}$ isomer[15] (tent.)
89	265	$C_{24}H_{18}$ isomer[16] (tent.)
90	265	$C_{21}H_{16}$ isomer[11] (tent.)
91	265	C_4 alkyl $C_{18}H_{12}$ isomer[6] (tent.)
92	265	$C_{21}H_{14}$ isomer[15] (tent.)
93	265	$C_{22}H_{18}$ isomer[17] (tent.)
94	265	unknown
95	265	methyl $C_{20}H_{12}$ isomer[9] (tent.)
96	265	unknown

1. $C_{12}H_{10}$ isomers include biphenyl and acenaphthene.
2. $C_{14}H_{10}$ isomers include diphenylacetylene, phenanthrene and anthracene.
3. $C_{16}H_{10}$ isomers include fluoranthene, pyrene, benz[a]acenaphthene and benz[*e*] acenaphthene.
4. $C_{17}H_{12}$ isomers include benzofluorene isomers and methyl $C_{16}H_{10}$ isomers.
5. $C_{18}H_{10}$ isomers include 1,10-benzfluoranthene, 3,4-cyclopentapyrene and 1,10-benzoaceanthrylene.
6. $C_{18}H_{12}$ isomers include benzanthracene isomers, benzophenanthrene isomers, triphenylene and chrysene.
7. $C_{19}H_{14}$ isomers include methyl $C_{18}H_{12}$ isomers.
8. $C_{22}H_{12}$ isomers include 1,12-benzperylene; 2,3-o-phenylenepyrene; anthanthrene and indeno[1,2,3-*cd*]pyrene.
9. $C_{20}H_{12}$ isomers include perylene; benzfluoranthene isomers; benzpyrene isomers and benzaceanthrylene isomers.
10. $C_{21}H_{20}$ isomers include C_3 alkyl terphenyl isomers; C_3 alkyl styrylnaphthalene isomers and triphenyl C_3 alkane isomers.
11. $C_{21}H_{16}$ isomers include diphenylindene isomers; methylbenzaceanthrene isomers; methylbenzilidine fluorene isomers and dinaphthylmethane isomers.
12. $C_{20}H_{14}$ isomers include acenaphthanthracene; phenylanthracene isomers; binaphthyl isomers; benzaceanthrene isomers; indenofluorene isomers and 9-benzylidene fluorene.
13. $C_{21}H_{18}$ isomers include dihydromethyl $C_{20}H_{14}$ isomers, tetrahydrocyclohepta-$C_{16}H_{10}$ isomers and methyl $C_{20}H_{16}$ isomers.
14. $C_{23}H_{14}$ isomers include methyl $C_{22}H_{12}$ isomers.
15. $C_{21}H_{14}$ isomers include methyl $C_{20}H_{12}$ isomers.
16. $C_{22}H_{18}$ isomers include triphenylbenzene isomers (quaterphenyls)
17. $C_{22}H_{18}$ isomers include dihydromethylcycloheptapyrene isomers; C_{22} alkyl $C_{20}H_{14}$ isomers and methyl $C_{21}H_{16}$ isomers.

Table D-3. COMPOUNDS IDENTIFIED IN PARAFFIN FRACTION OF <1.7 μ AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV (TRIP 3, P1/L1)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	115	undecane (tent.)
2	118	dimethylundecane (tent.)
3	123	an alkane
4	124	an alkane
5	125	an alkane
6	129	n-dodecane
7	131	an alkane
8	165	di-t-butyl-o-benzoquinone isomer + di-t-butyl-p-benzoquinone isomer
9	176	an alkane
10	$\sim$215-250	alkanes + alkenes
11	265	a phthalate (bkg.)
12	265	$C_{26}H_{54}$ alkane
13	265	$C_{27}H_{48}$ alkene
14	265	$C_{27}H_{56}$ alkane
15	265	$C_{28}H_{50}$ alkene
16	265	unknown
17	265	$C_{29}H_{52}$ arene
18	265	$C_{30}H_{34}$ arene
19	265	mixture of alkanes and alkenes
20	265	$C_{29}H_{52}$ arene
21	265	$C_{29}H_{52}$ arene
22	265	$C_{30}H_{54}$ arene
23	265	a phthalate (bkg.)
24	265	$C_{29}H_{60}$ alkane or $C_{30}H_{48}$ alkene
25	265	$C_{30}H_{54}$ arene
26	265	$C_{26}H_{54}$ alkene (tent.)
27	265	a phthalate (tent.)
28	265	unknown
29	265	$C_{30}H_{62}$ alkane
30	265	$C_{30}H_{30}$ arene (tent.)
31	265	arene(s)

Table D-4. COMPOUNDS IDENTIFIED IN BASE FRACTION OF <1.7 μ AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(TRIP 3, P1/L1)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	125	naphthalene (tent.)	10	198	p-nonylphenol
2	143	quinoline (tent.)	11	201	C_9 alkyl phenol
3	156	nicotine (tent.)	12	203	C_9 alkyl phenol
4	164	C_2 alkyl quinoline (tent.)	13	206	$C_{13}H_9N$ isomer
5	170	di-t-butylphenol	14	210	$C_{13}H_9N$ isomer
6	183	2,2,4-trimethylpenta-1,3-diol	15	211	caffeine (tent.)
		di-isobutyrate (bkg.)	16	213	a phthalate (bkg.)
7	191	C_9 alkyl phenol (tent.)	17	225	a phthalate ester (bkg.)
8	195	unknown	18	233	2,5-diphenyl oxazole
9	196	C_9 alkyl phenol	19*	265	dioctyladipate (bkg?)

*Unlabelled peaks beyond file position 400 are phthalates (bkg.)

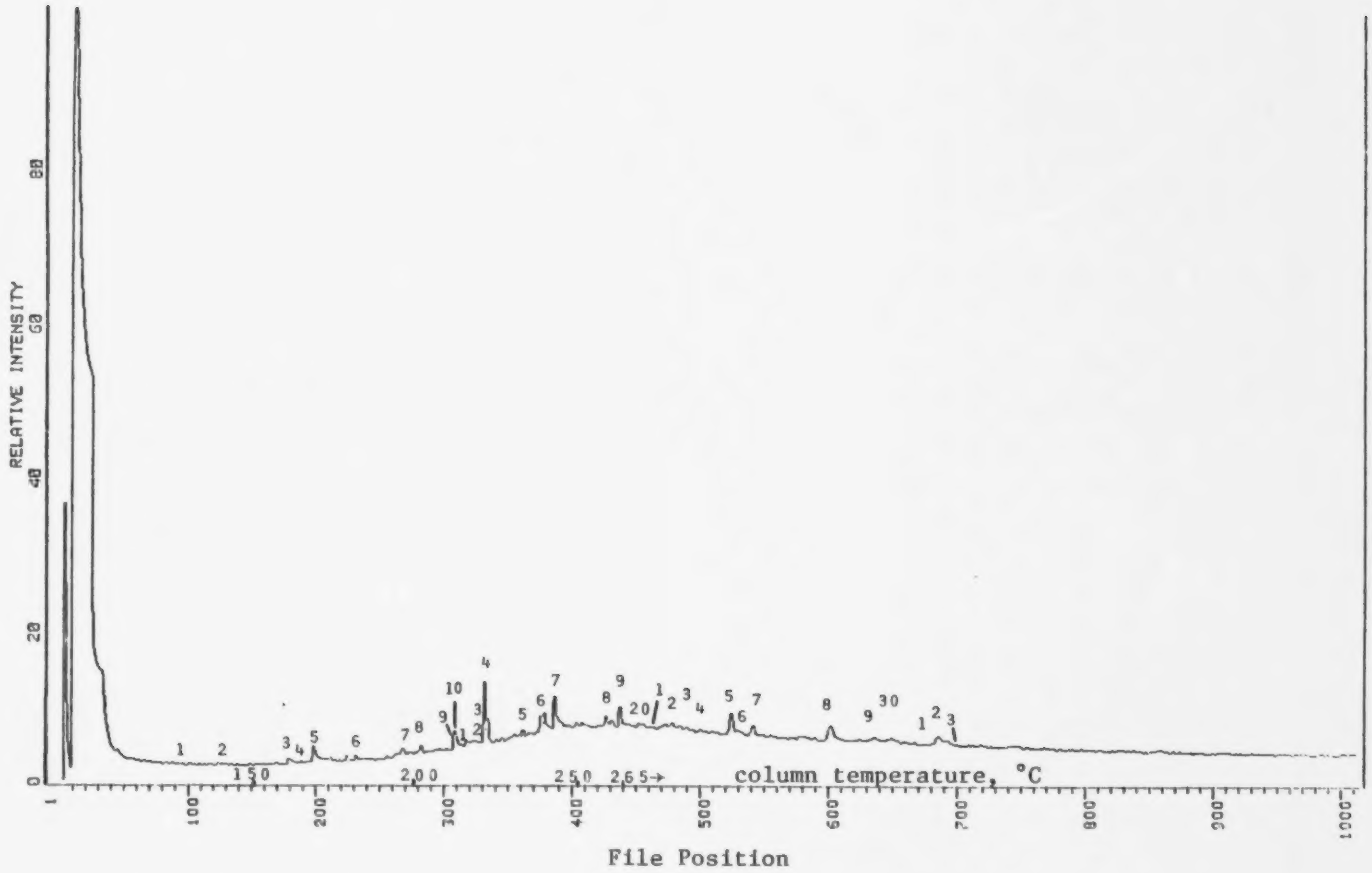


Figure D-1. Total ion current chromatogram of EC/MS/COMP Analysis of Polar Neutral Fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

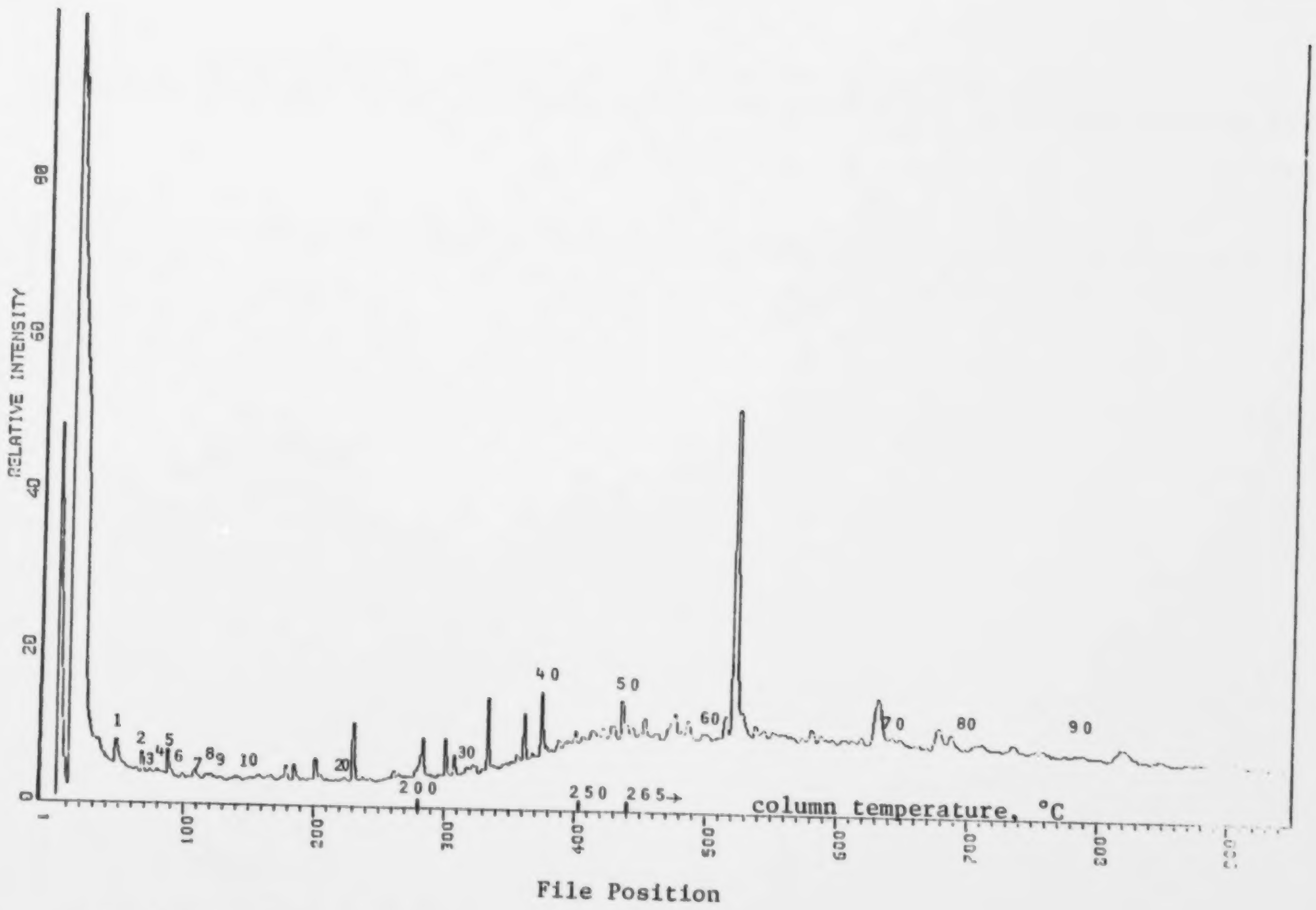


Figure D-2.. Total ion current chromatogram of GC/MS/COMP analysis of PNA fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

Reproduced from
best available copy.

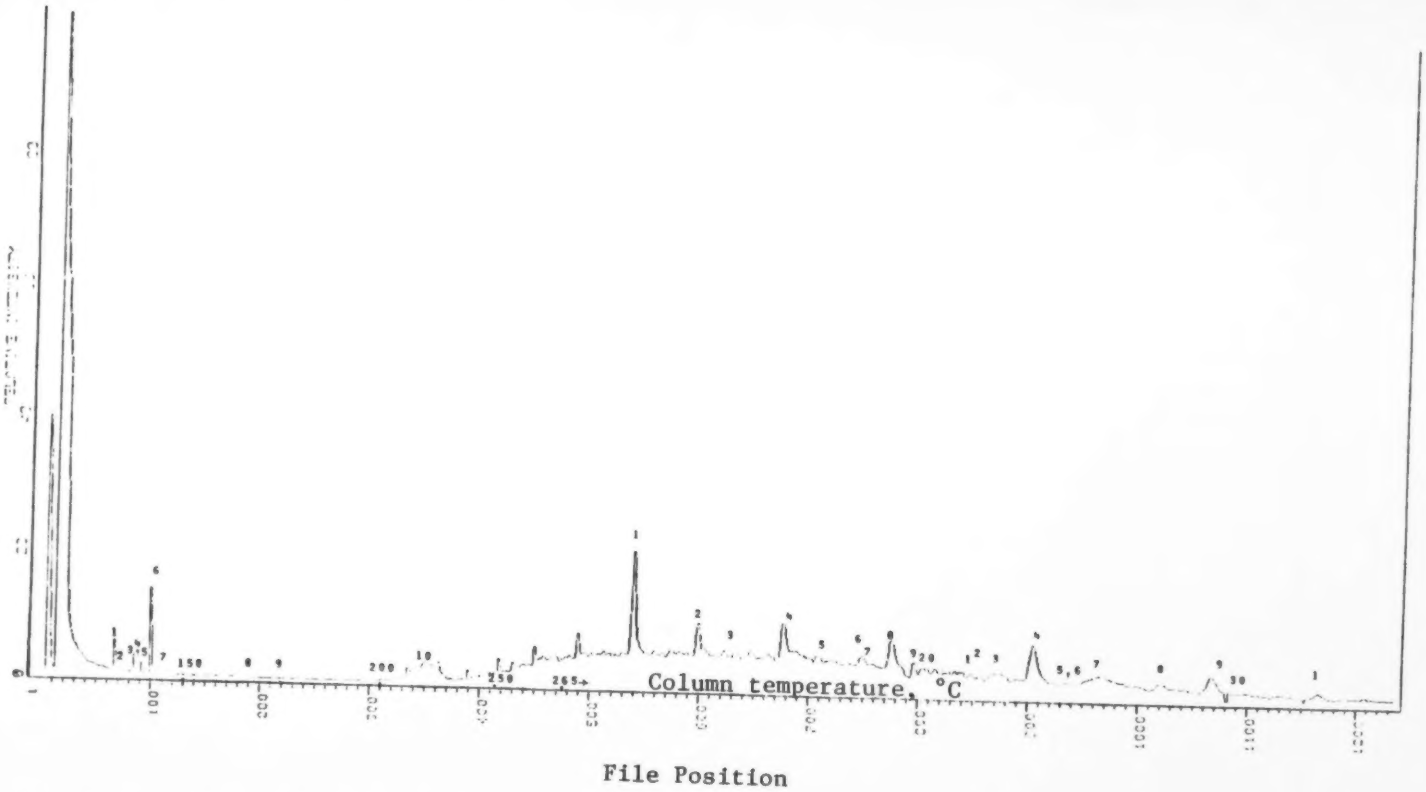


Figure D-3. Total ion current chromatogram of GC/MS/COMP analysis of paraffin fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

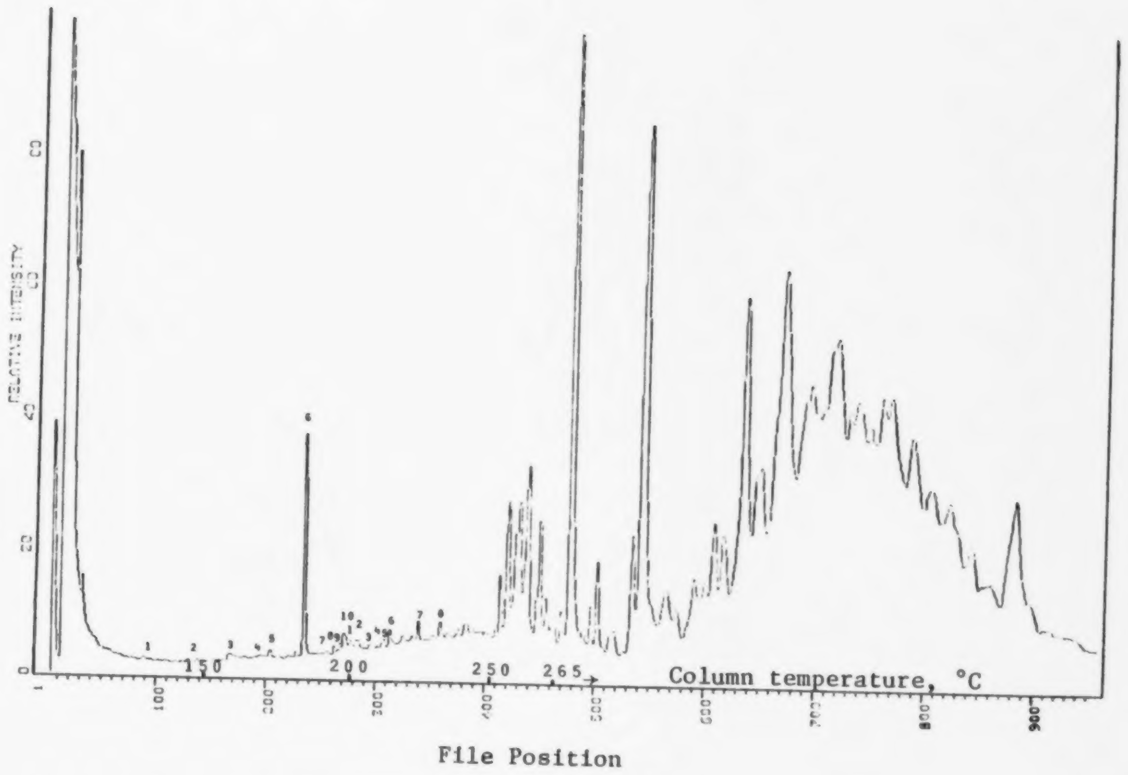


Figure D-4. Total ion current chromatogram of GC/MS/COMP analysis of base fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

APPENDIX E

VOLATILE AND VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA

Table E-1. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P1/L4).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	52	propane (tent.)
	52	isobutane (tent.)
	52	butene isomer
3	53	n-butane
	54	butene isomer
4	54	acetaldehyde
	56	C_5H_{10} isomer (tent.)
5	57	isopentane
6	58	acetone
7	59	n-pentane
7A	60	diethyl ether
8	61	vinylidene chloride
9	61	methylene chloride
10A	63	CS_2
10B	65	C_4H_8O isomer
10C	67	C_5H_{10} isomer
11	68	2-methylpentane
12	70	3-methylpentane
13	71	hexafluorobenzene (es)
14	72	n-hexane
15	73	chloroform
16	76	perfluorotoluene (es)
16A	78	methylcyclopentane
16B	82	benzene
16C	84	cyclohexane
16D	85	C_7H_{16} isomer
16E	86	C_7H_{16} isomer
17	89	C_8H_{18} isomer
18	94	acetic acid
19	103	toluene
19A	107	C_8H_{18} isomer
20	109	C_8H_{16} isomer
21	111	C_8H_{16} isomer
22	113	C_8H_{16} isomer

Table E-2. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P2/L5).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	52	C_4H_8 isomer + propane (tent.)
3	53	*n*-butane
3A	54	C_4H_8 isomer
3B	55	acetaldehyde
4	58	isopentane
4B	59	propanal
4C	59	acetone
4D	60	*n*-pentane
4E	60	diethyl ether
4F	61	vinylidene chloride
5	62	methylene chloride
6A	64	CS_2
6B	67	C_4H_6O isomer
7	68	2-methylpentane
7A	70	*n*-butanal
8	71	3-methylpentane
9	72	hexafluorobenzene (eI)
10	73	*n*-hexane
10A	74	chloroform
10B	75	$C_5H_{10}O$ isomer
11	77	perfluorotoluene (eI)
12	79	methylcyclopentane
13	83	benzene
14	85	cyclohexane
15	88	*n*-pentanal
16A	92	*n*-heptane
16B	95	C_7H_{14} isomer
17	105	toluene
17A	106	C_8H_{18} isomer (tent.)
17B	109	$C_6H_{12}O$ isomer
18	110	*n*-hexanal
18A	111	C_8H_{16} isomer
19	113	*n*-octane
20	117	C_8H_{16} isomer (tent.)

Table E-3. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P3/L2).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	54	C_4H_8 isomer
2B	56	n-butane
2C	57	acetaldehyde
2D	60	isopentane (tent.)
3	61	acetone
4	63	diethyl ether
5	64	vinylidene chloride
6	65	dichloromethane
8	71	2-methylpentane
9	74	3-methylpentane + n-butanal
9A	75	C_6H_{12} isomer
10	76	hexafluorobenzene (eI)
11	77	n-hexane
12	78	chloroform
13	79	ethyl acetate
14	81	perfluorotoluene (eI)
14A	82	methylcyclopentane
15	87	benzene
15A	87	carbon tetrachloride
15B	88	cyclohexane
15C	90	C_7H_{14} isomer (tent.)
16	91	acetic acid
17	93	pentanal (tent.)
18	96	n-heptane
18A	101	C_7H_{14} isomer
19	109	toluene
19A	110	C_8H_{18} isomer
19B	111	C_8H_{18} isomer
19C	113	C_8H_{16} isomer
20	114	n-hexanal
20A	115	C_8H_{16} isomer
21	117	n-octane
22	119	tetrachloroethylene
22A	123	C_8H_{16} isomer
22B	126	unsat. hydrocarbon
23	129	ethylbenzene
23A	130	C_9H_{18} isomer
24	131	xylene + C_9H_{20} isomers
24A	134	C_9H_{20} isomer
24B	134	styrene
25	135	o-xylene + n-heptanal
25A	136	C_9H_{20} isomer
25B	137	C_9H_{18} isomer
26	138	n-nonane
27	141	$C_{10}H_{22}$ isomer
28	145	$C_{10}H_{22}$ isomer
28A	148	$C_{10}H_{16}$ isomer
29	146	benzaldehyde
29A	147	n-propylbenzene
30	148	ethyltoluene isomer
30A	149	$C_8H_{16}O$ isomer
30B	149	phenol
31	150	$C_{11}H_{24}$ isomer
31A	151	$C_{10}H_{20}$ isomer
31B	151	$C_8H_{16}O$ isomer
32	152	$C_{11}H_{24}$ isomer
33	153	n-octanal
34	154	1,2,4-trimethylbenzene
34A	155	$C_{10}H_{20}$ isomer
35	156	n-decane
35A	157	dichlorobenzene isomer (tent.)
35B	159	$C_{11}H_{24}$ isomer
35C	160	1,2,3-trimethylbenzene
36	160	$C_{11}H_{24}$ isomer
36A	162	indan
37	164	C_4-alkyl benzene + $C_{12}H_{26}$ isomers
38	165	acetophenone
38A	166	cresol isomer
38B	166	$C_9H_{18}O$ isomer
38C	168	sat. hydrocarbon
38D	169	C_4-alkyl benzene isomer
38E	170	$C_{11}H_{22}$ isomer
38F	170	C_4-alkyl benzene isomer
39	171	n-nonanal
40	173	n-undecane
40A	174	$C_{11}H_{20}$ isomer (tent.)
41	178	dimethylphenol isomer
42	181	C_2-alkyl phenol isomer
43	183	C_2-alkyl phenol isomer
43A	185	C_5-alkyl benzene isomer
43B	185	$C_{10}H_{20}O$ isomer
44	186	C_3-alkyl phenol isomer
44A	187	naphthalene
45	188	n-decanal
45A	189	$C_{12}H_{24}$ isomer
46	189	n-dodecane
46A	190	C_2-alkyl phenol isomer
46B	191	C_3-alkyl phenol isomer
46C	193	C_3-alkyl phenol isomer
47	194	unknown

(continued)

Table E-3. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
48	195	unknown
48A	201	$C_{11}H_{22}O$ isomer
49	203	*n*-undecanal
49A	204	$C_{13}H_{26}$ isomer
50	204	*n*-tridecane
50A	205	β-methylnaphthalene
51	206	unknown
52	211	$C_{14}H_{30}$ isomer (tent.)
53	213	alkyl butyrate (BKG)
54	214	alkyl isobutyrate (BKG)
54A	216	C_6-alkyl phenol
55	217	*n*-tetradecane
55A	228	$C_{12}H_{24}O$ isomer (tent.)
56	229	$C_{15}H_{30}$ isomer
57	230	*n*-pentadecane
58	232	unknown

Table E-4. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P3/L6).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2A	52	C_4H_8 isomer
3	53	*n*-butane
4	54	C_4H_8 isomer
5	57	isopentane
6A	58	acetone
7	59	*n*-pentane
8	61	vinylidene chloride
9	61	methylene chloride
11	63	CS_2
12	67	2-methylpentane
12A	69	*n*-butanal
12B	69	methyl vinyl ketone
13	70	3-methylpentane
13A	70	methyl ethyl ketone
14	71	hexafluorobenzene (es)
15	72	*n*-hexane
15A	73	chloroform
16	76	perfluorotoluene (es)
17	77	methylcyclopentane
17A	81	$C_5H_{10}O$ isomer (tent.)
18	82	benzene
19	84	cyclohexane
19A	86	*n*-heptane (tent.)

Table E-5. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P3/L6).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
5	53	propane
5A	54	butene isomer
5B	54	*n*-butane
6	56	acetaldehyde
6A	59	isopentane
7	61	acetone
7A	65	dichloroethylene isomer (tent.)
8	65	dichloromethane
9A	71	C_4H_6O isomer
10	72	2-methylpentane
11	75	3-methylpentane
11A	76	C_6H_{12} isomer
12	76	hexafluorobenzene (eI)
13	77	*n*-hexane
14	78	chloroform
15	82	perfluorotoluene (eI)
15A	83	methylcyclopentane
15B	85	1,1,1-trichloroethane
15C	87	C_6H_{10} isomer
16	88	benzene
16A	88	carbon tetrachloride (tent.)
16B	89	cyclohexane
17	90	acetic acid + C_7H_{16} isomer
18	92	3-methylhexane
18A	94	*n*-pentanal
19	95	C_8H_{18} isomer
19A	96	C_7H_{14} isomer
20	97	*n*-heptane
20A	100	C_8H_{18} isomer
20B	103	methylcyclohexane
20C	104	C_8H_{18} isomer
20D	105	$C_6H_{12}O$ isomer
21	110	toluene
22	111	C_8H_{18} isomer
23	113	C_8H_{18} isomer
23A	114	C_8H_{16} isomer
24	115	*n*-hexanal
24A	116	C_8H_{16} isomer
25	118	*n*-octane
26	119	tetrachloroethylene
26A	124	C_9H_{20} isomer
26B	126	C_8H_{16} + C_9H_{20} isomers
26C	128	C_9H_{18} isomer
26D	128	$C_7H_{14}O$ aldehyde isomer
27	129	ethylbenzene
28	131	xylene isomer
29	133	C_9H_{20} isomer
29A	134	$C_7H_{14}O$ isomer
29B	134	*n*-heptaldehyde (tent.)
29C	135	styrene
30	136	*o*-xylene
30A	137	C_9H_{18} isomer
31	138	*n*-nonane
31A	140	C_9H_{18} isomer (tent.)
32	142	isopropylbenzene + $C_{10}H_{22}$ isomer
33	145	C_3-alkyl cyclohexane + $C_{10}H_{22}$ isomers
33A	146	$C_{10}H_{16}$ isomer
34	147	benzaldehyde
34A	148	*n*-propylbenzene
35	149	ethyltoluene isomer
35A	150	$C_{10}H_{22}$ isomer
36	150	1,3,5-trimethylbenzene + phenol
36A	151	$C_{11}H_{24}$ isomer
36B	152	$C_{10}H_{22}$ isomer
36C	152	*o*-ethyltoluene
37	154	*n*-octanal
38	155	1,2,4-trimethylbenzene
38A	156	$C_{10}H_{20}$ isomer
39	157	*n*-decane
39A	158	dichlorobenzene isomer
39B	158	C_4-alkyl benzene isomer
39C	159	$C_{10}H_{20}$ isomer
39D	160	C_4-alkyl benzene isomer
40	161	1,2,3-trimethylbenzene
40A	161	$C_{11}H_{24}$ isomer
40B	163	indan
40C	164	$C_{10}H_{20}$ isomer
40D	165	C_4-alkyl benzene isomer
40E	165	C_4-alkyl benzene isomer
41	166	acetophenone
41A	166	C_4-alkyl benzene isomer
41B	167	cresol isomer
41C	167	$C_{11}H_{24}$ isomer
41D	168	$C_{11}H_{22}$ isomer
41E	168	$C_{11}H_{24}$ isomer
41F	170	C_4-alkyl benzene isomer
41G	170	$C_9H_{18}O$ isomer
41H	171	C_4-alkyl benzene isomer

(continued)

Table E-5. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
42	172	*n*-nonanal
42A	171	$C_{11}H_{22}$ isomer
43	174	*n*-undecane
43A	175	C_4-alkyl benzene isomer
43B	176	$C_{11}H_{22}$ isomer
43C	177	C_4-alkyl benzene isomer
43D	177	tetramethylbenzene isomer
43E	178	$C_{12}H_{26}$ isomer
44	179	dimethylphenol isomer
44A	181	C_4H_7-benzene + C_5-alkyl benzene isomers
44B	181	$C_{11}H_{22}$ isomer
45	182	ethylphenol isomer
45A	183	C_4-alkyl benzene isomer
46	184	dimethylphenol isomer
46A	185	C_4-alkyl benzene isomer
47	186	C_3-alkyl phenol isomer
47A	186	$C_{12}H_{24}$ isomer
47B	187	naphthalene
48	188	*n*-decanal
48A	189	C_5-alkyl benzene isomer
49	190	*n*-dodecane
49A	191	C_3-alkyl phenol isomer
49B	193	C_3-alkyl phenol isomer
49C	198	$C_{13}H_{28}$ isomer
50	204	*n*-undecanal
51	205	*n*-tridecane
51A	205	β-methylnaphthalene
51B	206	unsat. hydrocarbon
51C	208	α-methylnaphthalene
52	213	alkyl butyrate
53	215	alkyl butyrate
53A	216	biphenyl
53B	217	C_6-alkyl phenol isomer
54	218	*n*-tetradecane
54A	221	C_2-alkyl naphthalene isomer (tent.)
54B	230	$C_{15}H_{30}$ isomer
55	231	*n*-pentadecane
56	233	unknown
57	240	diethyl phthalate
57A	240	$C_{16}H_{32}$ isomer
58A	240	*n*-hexadecane
58B	240	benzophenone

Table E-6. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 2, P2/L3).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	55	acetaldehyde
2B	57	*n*-butane
3	59	acetone
3A	61	diethyl ether (tent.)
3B	62	dichloroethylene isomer
4	63	dichloromethane
6	65	CS_2
6A	69	C_5H_{10} isomer
7	70	2-methylpentane
7A	71	C_3H_8O isomer
7B	71	C_4H_8O isomer
7C	72	3-methylpentane
7D	72	C_6H_{12} isomer
7E	73	methyl ethyl ketone
8	73	hexafluorobenzene (eS)
9	74	*n*-hexane
10	75	chloroform
10A	76	ethyl acetate
10B	77	C_6H_{12} isomer
11	78	perfluorotoluene (eS)
12	79	methylcyclopentane
12A	80	1,2-dichloroethane (tent.)
13	81	1,1,1-trichloroethane
14	83	benzene
14A	84	carbon tetrachloride
14B	85	cyclohexane
15	85	2-methylhexane
15A	86	2,3-dimethylpentane
16	87	3-methylhexane
16A	88	pentanal
16B	89	C_7H_{14} isomer
17	90	trichloroethylene
17A	90	C_8H_{18} isomer (tent.)
18	92	*n*-heptane
18A	93	C_7H_{14} isomer
18B	96	C_8H_{18} isomer
19	97	methylcyclohexane
20	97	acetic acid
20A	98	$C_7H_{14}O$ isomer (tent.)
20B	101	C_8H_{16} isomer
21	103	toluene
22	105	C_8H_{18} isomer
23	106	C_8H_{18} isomer
23A	107	C_8H_{16} isomer
23B	108	C_8H_{16} isomer
24	109	C_9H_{20} isomer
24A	111	C_8H_{16} isomer
25	112	*n*-octane
25A	113	C_8H_{16} isomer
26	113	tetrachloroethylene
26A	117	C_9H_{20} isomer
27	118	C_9H_{20} isomer
28	119	ethylcyclohexane or C_8H_{16} isomer
28A	120	C_9H_{20} isomer
28B	120	C_9H_{18} isomer
28C	122	C_9H_{18} isomer
29	123	ethylbenzene
29A	124	C_9H_{18} isomer
29B	124	C_9H_{20} isomer
30	125	xylene isomer
30A	125	C_9H_{20} isomer
31	127	C_9H_{20} isomer
31A	127	$C_7H_{14}O$ isomer (tent.)
32	128	C_9H_{20} isomer
32A	129	styrene
32B	129	C_9H_{18} isomer
33	130	*o*-xylene
33A	131	C_9H_{18} isomer
34	132	*n*-nonane
34A	134	C_9H_{18} isomer
35	135	$C_{10}H_{22}$ isomer
36	136	$C_{10}H_{22}$ isomer + isopropylbenzene
37	137	$C_{10}H_{22}$ isomer
37A	138	$C_{10}H_{20}$ isomer
38	139	$C_{10}H_{22}$ + C_3-alkyl cyclohexane isomers
39	140	$C_{10}H_{16}$ isomer
40	141	benzaldehyde
40A	141	*n*-propylbenzene
40B	142	$C_{10}H_{20}$ isomer
41	143	ethyltoluene isomer
41A	144	1,3,5-trimethylbenzene
42	144	$C_{11}H_{24}$ isomer
42A	145	phenol
42B	145	$C_{10}H_{22}$ isomer
43	146	*o*-ethyltoluene
44	147	sat. hydrocarbon
45	147	$C_{10}H_{16}$ isomer
45A	148	$C_{10}H_{20}$ isomer

(continued)

Table E-6. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
46	148	1,2,4-trimethylbenzene
46A	149	$C_{10}H_{20}$ isomer
47	150	n-decane
47A	151	dichlorobenzene isomer
48	151	$C_{11}H_{24}$ isomer (tent.)
48A	152	C_4-alkyl benzene isomer
48B	153	C_4-alkyl benzene isomer
48C	153	1,2,3-trimethylbenzene
49	154	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
50	155	$C_{11}H_{24}$ isomer
50A	156	$C_{10}H_{16}$ isomer
50B	156	indan
51	157	$C_{11}H_{24}$ isomer
51A	157	$C_{10}H_{20}$ isomer
52	158	$C_{11}H_{24}$ isomer
52A	158	C_4-alkyl benzene isomer
53	159	acetophenone
53A	160	cresol isomer
53B	160	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
54	161	$C_{11}H_{24}$ isomer
54A	161	$C_{11}H_{22}$ isomer
54B	163	C_4-alkyl benzene isomer
54C	163	$C_{11}H_{22}$ isomer
55	164	C_4-alkyl benzene isomer
55A	165	C_4H_7-benzene isomer
56	165	n-nonanal
56A	166	$C_{11}H_{22}$ isomer
57	167	n-undecane
57A	167	C_5-alkyl benzene isomer
57B	168	$C_{11}H_{22}$ isomer
58	170	C_4-alkyl benzene isomer
59	172	dimethylphenol isomer
59A	173	C_5-alkyl benzene isomer
59B	173	C_4H_7-benzene isomer
60	174	C_2-alkyl phenol isomer
60A	175	C_4H_7-benzene isomer (tent.)
60B	176	C_4-alkyl benzene isomer
60C	176	C_5-alkyl benzene isomer
61	176	C_2-alkyl phenol isomer
61A	177	C_5-alkyl benzene isomer
61B	179	C_2-alkyl phenol isomer
62	179	C_3-alkyl phenol isomer
63	181	naphthalene + $C_{12}H_{24}$ isomer
64	183	n-dodecane
64A	183	$C_{13}H_{26}$ isomer
65	184	C_3-alkyl phenol isomer
66	187	unknown
66A	189	$C_{13}H_{26}$ isomer
66B	195	$C_{13}H_{26}$ isomer
67	196	n-tridecane
67A	197	β-methylnaphthalene
67B	198	$C_{13}H_{26}$ isomer
67C	199	α-methylnaphthalene
67D	204	$C_{13}H_{26}$ isomer
68	205	alkyl butyrate
69	207	alkyl butyrate
69A	208	$C_{12}H_{24}O$ isomer
69B	208	biphenyl (tent.)
69C	209	C_6-alkyl phenol isomer
70	209	$C_{14}H_{28}$ isomer
71	210	sat. hydrocarbon
71A	212	C_2-alkyl naphthalene isomer
73	219	unsat. hydrocarbon
73A	221	$C_{13}H_{26}O$ isomer (tent.)
73B	222	$C_{15}H_{30}$ isomer
74	223	n-pentadecane
75	225	unknown
76	232	diethyl phthalate
76A	234	$C_{14}H_{28}O$ isomer
77A	236	$C_{16}H_{32}$ isomer
77B	240	$C_{15}H_{30}O$ isomer (tent.)
78	240	n-heptadecane

Table E-7. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 2, P3/L5).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
4	51	*n*-propane (tent.)
4A	51	butene isomer
5	52	*n*-butane
6	53	acetaldehyde
6A	55	isopentane
7	58	acetone
7A	60	diethyl ether (tent.)
8	61	vinylidene chloride
9	62	dichloromethane
10A	66	C_4H_8O isomer
11	68	cyclopentane
11A	68	2-methylpentane
11B	69	methyl isopropyl ketone (tent.)
12	70	*n*-butanal
12A	71	3-methylpentane
13	72	hexafluorobenzene (eS)
14	73	*n*-hexane
14A	74	chloroform
15	75	ethyl acetate
16	77	perfluorotoluene (eS)
17	78	methylcyclopentane
18	83	benzene
18A	84	carbon tetrachloride
19	84	cyclohexane
19A	85	2-methylhexane
19B	86	2,3-dimethylpentane
20	87	3-methylhexane + C_7H_{14} isomer
20A	88	acetic acid (tent.)
21	90	C_8H_{18} isomer
22	91	*n*-heptane
22A	93	C_7H_{14} isomer (tent.)
22B	96	C_8H_{18} isomer
23	97	methylcyclohexane
23A	99	C_8H_{18} isomer
24	104	toluene
24A	105	C_8H_{18} isomer
24B	107	C_8H_{18} isomer
25	109	*n*-hexanal (tent.) + C_8H_{16} isomer
26	112	*n*-octane
27	113	tetrachloroethylene
27A	123	ethylbenzene
28	125	xylene isomer
28A	126	C_9H_{20} isomer (tent.)
28B	128	$C_7H_{14}O$ isomer (tent.)
28C	129	styrene
29	130	*o*-xylene + C_9H_{20} isomer
29A	131	C_9H_{18} isomer (tent.)
30	132	*n*-nonane
31	136	$C_{10}H_{22}$ isomer
32	139	$C_{10}H_{22}$ isomer
33	140	$C_{10}H_{16}$ isomer
34	141	benzaldehyde
34A	143	ethyltoluene isomer
34B	144	$C_6H_{16}O$ isomer
34C	144	phenol + C_3-alkyl benzene isomer
35	145	$C_{11}H_{24}$ isomer
35A	146	C_3-alkyl benzene isomer
36	147	$C_{10}H_{22}$ isomer
36A	148	$C_{11}H_{24}$ isomer
37	149	*n*-octanal
37A	149	trimethylbenzene isomer
38	150	*n*-decane
38A	151	$C_{11}H_{24}$ isomer
38B	152	$C_{10}H_{20}$ isomer (tent.)
38C	154	$C_{11}H_{24}$ isomer
39	156	sat. hydrocarbon
40	159	$C_{11}H_{24}$ isomer
41	160	acetophenone
41A	161	cresol isomer
41B	162	$C_{12}H_{26}$ isomer (tent.)
41C	164	C_4-alkyl benzene isomer
41D	165	$C_9H_{18}O$ isomer
42	166	*n*-nonanal
42A	167	$C_{11}H_{22}$ isomer
43	168	*n*-undecane
44	173	dimethylphenol isomer
45	176	C_2-alkyl phenol isomer
45A	178	C_2-alkyl phenol isomer
45B	179	unsat. hydrocarbon
46	180	C_3-alkyl phenol isomer
46A	181	naphthalene (tent.)
47	182	*n*-decanal
48	183	*n*-dodecane
48A	185	C_3-alkyl phenol isomer
48B	186	$C_{12}H_{24}$ isomer
48C	187	C_3-alkyl phenol isomer
48D	191	unsat. hydrocarbon
48E	195	$C_{11}H_{22}O$ isomer
49	197	*n*-undecanal

(continued)

Table E-7. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
50	198	n-tridecane
50A	198	β-methylnaphthalene
50B	201	α-methylnaphthalene
50C	204	unsat. hydrocarbon
50D	205	unsat. hydrocarbon
51	208	alkyl butyrate
51A	209	$C_{12}H_{24}O$ isomer
51B	211	unsat. hydrocarbon
52	212	n-tetradecane
53	217	unknown
53A	221	unsat. hydrocarbon
53B	222	$C_{13}H_{26}O$ isomer
54	223	$C_{15}H_{30}$ isomer
55	224	n-pentadecane
56	226	unknown
57	233	diethyl phthalate
57A	235	$C_{16}H_{32}$ isomer
58A	236	n-hexadecane (tent.)
58B	240	benzophenone
58C	240	$C_{15}H_{30}O$ isomer
58D	240	$C_{17}H_{34}$ isomer
58E	240	n-heptadecane

Table E-8. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 3, P1/L9).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
3A	53	propane
3B	53	propylene
4	54	isobutane
4A	55	C_4H_8 isomer
5	56	acetaldehyde
5A	57	C_4H_8 isomer
6	58	n-butane
7	60	isopentane
8	61	acetone
8A	64	diethyl ether (tent.)
9	65	methylene chloride
10A	67	CS_2
12	72	2-methylpentane
13	75	3-methylpentane
14	76	hexafluorobenzene (eS)
15	77	n-hexane
15A	78	chloroform

Table E-9. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 3, P2/L8).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
3A	51	propane (tent)
5	53	C_4H_{10} isomer
6	55	acetaldehyde
7	56	n-butane
8	58	isopentane
9	59	acetone
10	60	n-pentane
11	61	diethyl ether
12	62	Background peak
13	63	methylene chloride
16	67	C_6H_{14} isomer (tent)
16A	69	C_5H_{10} isomer
17	70	2-methylpentane
18	72	3-methylpentane
19	74	hexafluorobenzene (es)
20	75	n-hexane
20A	76	chloroform
21	77	methyl ethyl ketone (tent)
21A	78	ethyl acetate (tent)
22	79	perfluorotoluene (es)
23	80	methylcyclopentane
24	81	1,1,1-trichloroethane
24A	83	C_7H_{14} isomer
24B	84	C_6H_{10} isomer
25	85	benzene
25A	86	carbon tetrachloride (tent)
26	87	cyclohexane
27	87	2-methylhexane
27A	88	2,3-dimethylpentane
27B	88	acetic acid
28	89	3-methylhexane
29	91	n-pentanal
29A	91	C_7H_{14} isomer
30	92	C_8H_{18} isomer + trichloroethylene
31	94	n-heptane
32	95	C_7H_{12} isomer
33	97	unsat. hydrocarbon
34	99	methylcyclohexane
35	101	C_8H_{18} + $C_6H_{12}O$ isomers
36	105	C_8H_{18} isomer
37	106	toluene
38	108	C_8H_{18} isomer
39	109	C_8H_{18} isomer
39A	111	C_8H_{16} isomer
39B	111	$C_6H_{12}O$ isomer
40	112	hexanal
40A	113	C_8H_{16} isomer
41	114	n-octane
41A	115	C_8H_{16} isomer
42	116	tetrachloroethylene
43	118	C_8H_{16} isomer
43A	119	C_9H_{20} isomer
43B	121	C_9H_{20} isomer
43C	121	C_8H_{16} isomer
44	122	C_9H_{20} isomer + ethylcyclohexane
44A	123	C_9H_{18} isomer
45	126	ethylbenzene
45A	126	C_9H_{18} isomer
45B	127	C_9H_{20} isomer
46	127	xylene isomer
46A	128	C_9H_{20} isomer
47	129	C_9H_{20} isomer
47A	130	$C_7H_{14}O$ isomer
48	131	styrene
48A	131	n-heptanal
49	132	o-xylene
49A	133	C_9H_{18} isomer
50	134	n-nonane
50A	135	$C_{10}H_{22}$ isomer
50B	137	C_9H_{18} isomer
51	138	$C_{10}H_{22}$ isomer + isopropylbenzene
52	139	$C_8H_{16}O$ isomer
53	141	$C_{10}H_{22}$ isomer
54	142	$C_{10}H_{16}$ isomer
55	143	benzaldehyde
56	144	n-propylbenzene
57	145	ethyltoluene isomer
57A	146	phenol
57B	146	1,3,5-trimethylbenzene
58	147	$C_{10}H_{22}$ isomer
59	148	o-ethyltoluene
59A	149	$C_{10}H_{22}$ isomer
59B	149	$C_{11}H_{24}$ isomer
60	150	n-octanal isomer (tent)
60A	151	$C_{10}H_{20}$ isomer
61	151	1,2,4-trimethylbenzene
61A	152	$C_{10}H_{20}$ isomer
62	153	n-decane

(continued)

Table E-9. (cont'd.)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
62A	154	dichlorobenzene isomer
62B	154	C_4-alkyl benzene isomer
62C	155	$C_{11}H_{24}$ isomer
62D	156	C_4-alkyl benzene isomer
63	156	1,2,3-trimethylbenzene
63A	157	$C_{11}H_{24}$ isomer
63B	159	indan
63C	160	C_4-alkyl cyclohexane isomer
64	161	C_4-alkyl benzene isomer
64A	161	C_4-alkyl benzene isomer
65	162	acetophenone + C_4-alkyl benzene isomer
65A	163	cresol isomer
65B	163	$C_{11}H_{22}$ isomer
66	164	$C_{11}H_{24}$ isomer
66A	164	C_4-alkyl benzene isomer
66B	165	$C_{10}H_{18}$ isomer
67	166	$C_{11}H_{24}$ isomer
67A	167	C_4-alkyl benzene isomer
68	168	C_4-alkyl benzene isomer
69	169	*n*-nonanal
69A	170	$C_{11}H_{22}$ isomer
70	171	*n*-undecane
70A	172	C_4-alkyl benzene isomer
70B	172	$C_{11}H_{22}$ isomer
70C	174	C_4-alkyl benzene isomer
71	175	$C_{12}H_{24}$ isomer
72	176	C_2-alkyl phenol isomer
72A	177	C_5-alkyl benzene isomer
72B	178	C_5-alkyl benzene + C_4H_7 benzene isomers
72D	179	C_5-alkyl benzene isomer
72E	179	C_2-alkyl phenol isomer
73	180	C_4-alkyl benzene + $C_{12}H_{26}$ isomers
73A	181	$C_{12}H_{26}$ isomer
73B	183	C_5-alkyl benzene + $C_{12}H_{24}$ isomers
73C	183	C_2-alkyl phenol isomer
73D	184	C_2-alkyl phenol isomer
74	185	naphthalene + *n*-decanal
74A	186	$C_{12}H_{24}$ isomer
75	187	*n*-dodecane
75A	189	$C_{13}H_{28}$ isomer
75B	190	C_3-alkyl phenol isomer
76	192	unknown
76A	197	$C_{14}H_{30}$ isomer
76B	199	unsat. hydrocarbon
77	200	*n*-undecanal
78	201	*n*-tridecane
78A	202	β-methylnaphthalene
79	204	unknown
79A	204	α-methylnaphthalene
80	215	*n*-tetradecane
80A	228	unsat. hydrocarbon
80B	229	*n*-pentadecane
80C	230	$C_{15}H_{30}$ isomer
81	232	unknown
81A	237	unsat. hydrocarbon
81B	238	diethyl phthalate
81C	239	$C_{16}H_{34}$ isomer
82A	240	$C_{16}H_{34}$ isomer

Table E-10. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 3, P2/L9).

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	47	CO_2
3	52	C_4H_{10} isomer (tent)
3A	53	acetaldehyde
3B	55	SO_2
3C	57	isopentane
4	59	acetone
4A	60	n-pentane
4B	61	diethyl ether
4C	61	Background peak
5	62	methylene chloride
6A	64	CS_2
6B	68	C_5H_{10} isomer
7	69	2-methylpentane
8	71	3-methylpentane
8A	72	C_6H_{12} isomer
9	73	hexafluorobenzene (es)
10	74	n-hexane
10A	74	chloroform
10B	77	C_6H_{12} isomer
11	78	perfluorotoluene (es)
12	79	methylcyclopentane
12A	81	1,1,1-trichloroethane
13	84	benzene
13A	85	carbon tetrachloride
13B	85	cyclohexane
14	86	2-methylhexane
14A	87	2,3-dimethylpentane
15	88	3-methylhexane
15A	89	acetic acid
16	90	C_7H_{14} isomer
16A	90	C_7H_{14} isomer
17	91	trichloroethylene + C_8H_{18} isomer
18	93	n-heptane
18A	94	C_7H_{14} isomer
18B	96	C_7H_{14} isomer
18C	97	C_8H_{18} isomer
19	98	methylcyclohexane
19A	99	C_8H_{18} isomer
19B	100	$C_6H_{12}O$ isomer
20	100	C_8H_{18} isomer
20A	101	C_8H_{16} isomer
21	104	C_8H_{18} isomer
22	105	toluene
23	106	C_8H_{18} isomer
24	108	C_8H_{18} isomer
24A	110	C_8H_{16} isomer
25	110	C_8H_{13} isomer
25A	111	C_8H_{16} isomer
25B	113	C_8H_{16} isomer
26	113	n-octane
26A	114	C_8H_{16} isomer
27	115	tetrachloroethylene
27A	115	C_8H_{16} isomer
27B	117	C_9H_{20} isomer
28	119	C_9H_{20} isomer
28A	120	C_8H_{16} isomer
29	121	C_9H_{20} isomer
29A	122	C_9H_{18} isomer
30	124	ethylbenzene
30A	125	C_9H_{18} isomer
31	126	xylene
31A	126	C_9H_{20} isomer
32	127	C_9H_{20} isomer
32A	128	$C_7H_{14}O$ isomer (tent)
33	129	styrene
33A	129	C_9H_{18} isomer
34	130	o-xylene
34A	131	C_9H_{18} isomer
35	132	n-nonane
35A	134	$C_{10}H_{20}$ isomer
35B	135	C_9H_{18} isomer
36	136	isopropylbenzene + $C_{10}H_{22}$ isomer
37	137	$C_{10}H_{22}$ isomer
37A	138	C_9H_{16} isomer (tent)
37B	138	$C_{10}H_{22}$ isomer
38	139	$C_{10}H_{22}$ + C_3-alkyl cyclohexane isomer
38A	140	$C_{10}H_{16}$ isomer
39	141	benzaldehyde
40	142	n-propylbenzene
41	143	ethyltoluene isomer
41A	144	$C_{10}H_{22}$ isomer
42	144	1,3,5-trimethylbenzene
42A	145	$C_{10}H_{22}$ isomer
42B	145	$C_{10}H_{20}$ isomer
43	146	o-ethyltoluene
43A	147	$C_{11}H_{24}$ isomer
43B	148	$C_{10}H_{20}$ isomer
43C	148	n-octanal
43D	149	C_3H_5-benzene isomer

continued

Table E-10. (cont'd.)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
44	149	1,2,4-trimethylbenzene
44A	150	$C_{10}H_{20}$ isomer
45	151	n-decane
45A	152	dichlorobenzene isomer
45B	152	C_4-alkyl benzene isomer
45C	153	$C_{10}H_{20}$ isomer
45D	154	C_4-alkyl benzene isomer
46	154	1,2,3-trimethylbenzene
46A	155	$C_{11}H_{24}$ isomer
46B	156	$C_{11}H_{24}$ isomer
46C	157	indan
46D	158	C_4-alkyl cyclohexane isomer
46E	158	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
47	159	C_4-alkyl benzene isomer
48	160	acetophenone + C_4-alkyl benzene isomer
48A	161	$C_{11}H_{24}$ isomer
48B	162	$C_{11}H_{22}$ isomer
49	162	C_4-alkyl benzene isomer
49A	163	$C_{11}H_{24}$ isomer
50	164	C_4-alkyl benzene isomer
50A	164	$C_{11}H_{22}$ isomer
50B	165	C_4H_7-benzene isomer (tent)
51	165	C_4-alkyl benzene isomer
52	166	n-nonanal
52A	166	C_4-alkyl benzene isomer
52B	167	$C_{11}H_{22}$ isomer
53	168	n-undecane
53A	168	C_4-alkyl benzene isomer
53B	169	$C_{11}H_{22}$ isomer
53C	169	C_5-alkyl benzene isomer
53D	170	C_4-alkyl benzene isomer
54	171	tetramethylbenzene isomer
54A	172	$C_{12}H_{26}$ isomer
54B	172	$C_{11}H_{20}$ isomer
54C	173	C_5-alkyl benzene isomer
54D	174	C_5-alkyl benzene isomer
54E	175	C_4H_7-benzene isomer
54F	175	C_5-alkyl cyclohexane isomer
54G	176	C_5-alkyl benzene isomer
55	177	$C_{12}H_{26}$ + C_4-alkyl benzene isomers
55A	177	C_5-alkyl benzene isomer
55B	178	C_4alkyl benzene + $C_{12}H_{26}$
55C	179	C_5-alkyl benzene isomer
55D	180	$C_{12}H_{24}$ + alkyl benzene isomers
56	182	naphthalene
56A	182	n-decanal
56B	183	$C_{12}H_{24}$ isomer
56C	183	C_5-alkyl benzene isomer
57	184	n-dodecane
57A	185	C_5-alkyl benzene isomer
57B	186	$C_{13}H_{28}$ isomer
57C	187	C_6-alkyl benzene isomer (tent)
57D	190	$C_{13}H_{26}$ isomer
57E	192	$C_{13}H_{28}$ isomer
58	198	n-tridecane
58A	199	β-methylnaphthalene
58B	201	α-methylnaphthalene
58C	206	biphenyl (tent)
59	208	n-tetradecane
59A	210	$C_{14}H_{28}$ isomer
59B	216	$C_{16}H_{34}$ isomer
59C	217	unsat. hydrocarbon
59D	220	n-pentadecane
59E	221	$C_{15}H_{30}$ isomer
60	239	$C_{16}H_{34}$ isomer

APPENDIX F

SEMIVOLATILE COMPOUNDS IDENTIFIED IN AIR PARTICULATE COLLECTED IN SHENANDOAH VALLEY, VA

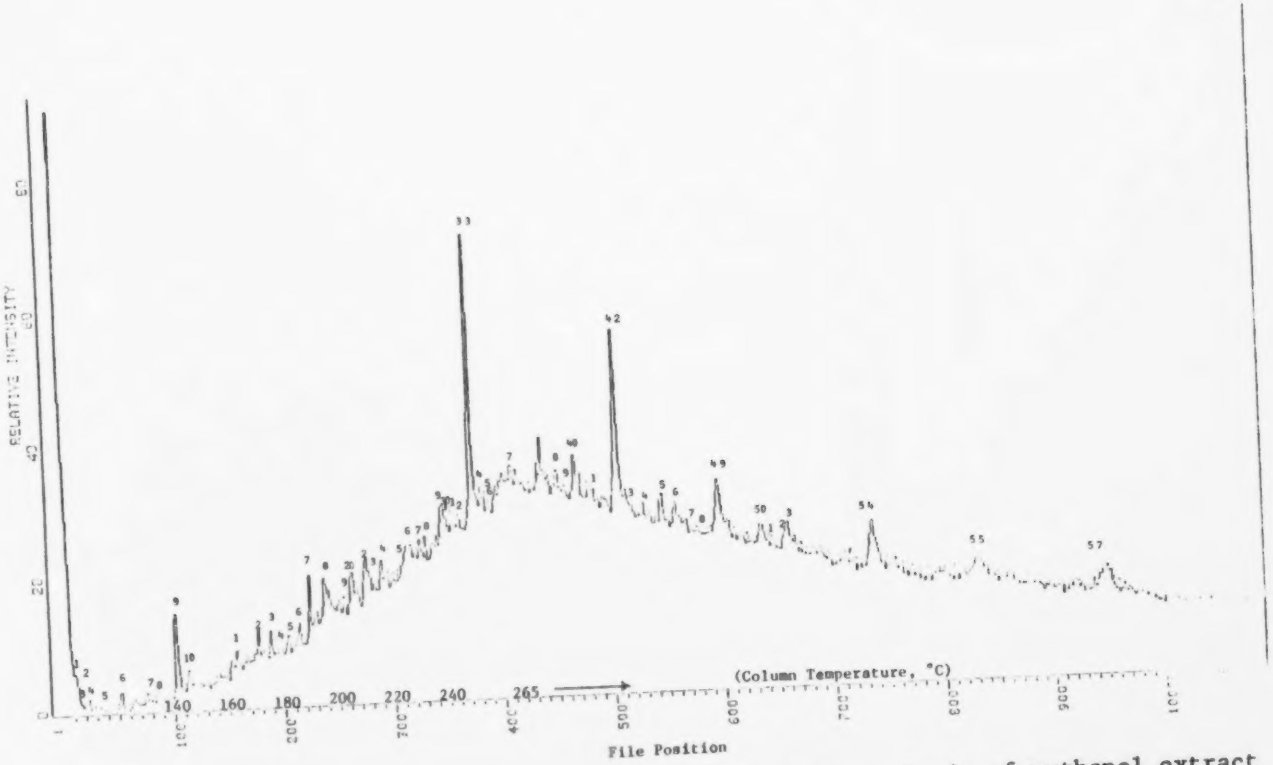


Figure F-1. Total ion current chromatogram of gc/ms/comp analysis of methanol extract of < 1.7 µ air particulate collected in Front Royal, VA (Trip 3, P1/L4).

Table F-1. COMPOUNDS IDENTIFIED IN METHANOL EXTRACT OF <1.7μ FRACTION OF AIR PARTICULATE COLLECTED IN FRONT ROYAL, VA (TRIP 3, P1/L4).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	100-107	dichloromethane (solvent)
2	104-106	toluene (solvent)
3	108	benzaldehyde
4	108.5	phenol
5	113	methylacetophenone isomer (tent.)
6	120.5	unknown
7	129	naphthalene (tent.)
8	134.5	benzothiazole (tent.)
9	140-142	unknown
10	145	methylnaphthalene (tent.) + phthalic anhydride
11	170.5	$(C_4H_9)_2$ benzoquinone isomer (tent.) + Si cmpd. (bkg.)
12	171	dibenzofuran (tent.)
13	175	unknown
14	177	di-butylcresol isomer (bkg.)
15	181	C_2 alkyl biphenyl isomer + Si cmpd. (bkg.)
16	185	a phthalate (bkg.)
17	189	unknown
18	195	4-hydroxy-3,5-dimethoxybenzaldehyde
19	202	unknown
20	204	methylxanthene isomer (tent.)
21	207	methylxanthene isomer (tent.)
22	211	$C_{14}H_{10}$ isomer(s)[1]
23	212	phenothiazine (tent.)
24	216	C_2 alkyl xanthene
25	224	9-fluorenone (tent.)
26	225	$C_{15}H_{12}$ isomer[2] (tent.)
27	231	unknown
28	232	a phthalate (bkg.)
29	238	naphthalic anhydride
30	239	C_2 alkyl $C_{18}H_{12}$ isomer[3] (tent.)
31	241	methylphenylindole isomer (tent.)
32	244	$C_{16}H_{10}$ isomer[4]
33	249	pyrene + pyrene-d_{10} (ext. std.)
34	252	Si cmpd. (bkg.)
35	254	Si cmpd. (bkg.)
36	255	Si cmpd. (bkg.)
37	265	Si cmpds. (bkg.) + phthalates (bkg.)
38	265	$C_{18}H_{10}$ isomer[5]
39	265	$C_{18}H_{14}$ isomer[6]
40	265	$C_{18}H_{12}$ isomer[3] + $C_{18}H_{10}$ isomer (tent.)
41	265	benzanthrone
42	265	a phthalate (bkg.)
43	265	$C_{19}H_{14}$ isomer[7]
44	265	$C_{19}H_{12}$ isomer[8] (tent.)
45	265	bkg.
46	265	unknown
47	265	C_2 alkyl $C_{18}H_{12}$ isomer[3] (tent.)
48	265	C_2 alkyl $C_{18}H_{10}$ isomer (tent.)
49	265	$C_{20}H_{12}$ isomer[9]
50	265	$C_{20}H_{12}$ isomer[9]
51	265	$C_{20}H_{12}$ isomer[9] + C_2 alkyl $C_{18}H_{10}$ isomer
52	265	C_3 alkyl $C_{18}H_{12}$ isomer[3] (tent.)
53	265	$C_{20}H_{12}$ isomer[9] (tent.)
54	265	$C_{19}H_{14}$ isomer[7] (tent.)
55	265	bkg.
56	265	$C_{22}H_{12}$ isomer[10]
57	265	$C_{22}H_{12}$ isomer[10]

Notes:

[1] $C_{14}H_{10}$ isomers include anthracene, phenanthrene, and diphenyl acetylene.

[2] $C_{15}H_{12}$ isomers include methylphenanthrene and methylanthracene.

[3] $C_{18}H_{12}$ isomers include chrysene, benzophenanthrene isomers, triphenylene, naphthalene, and benzanthracene isomers.

[4] $C_{16}H_{10}$ isomers include pyrene, fluoranthene, and diphenyldiacetylene.

[5] $C_{18}H_{10}$ isomers include 1,10-benzfluoranthene and 3,4-cyclopentapyrene.

[6] $C_{18}H_{14}$ isomers include terphenyl isomers, styrylnaphthalene isomers, and dihydrobenzanthracene isomers.

[7] $C_{19}H_{14}$ isomers include methyltriphenylene isomers, methylbenzanthracene isomers, methylchrysene isomers, methylbenzophenanthrene isomers, and 9-phenylfluorene.

[8] $C_{19}H_{12}$ isomers include methyl-1,10-benzfluoranthene isomers.

[9] $C_{20}H_{12}$ isomers include perylene, benzpyrene isomers, and benzfluoranthene isomers.

[10] $C_{22}H_{12}$ isomers include 1,12-benzperylene, anthanthrene, and 2,3-o-phenylenepyrene.

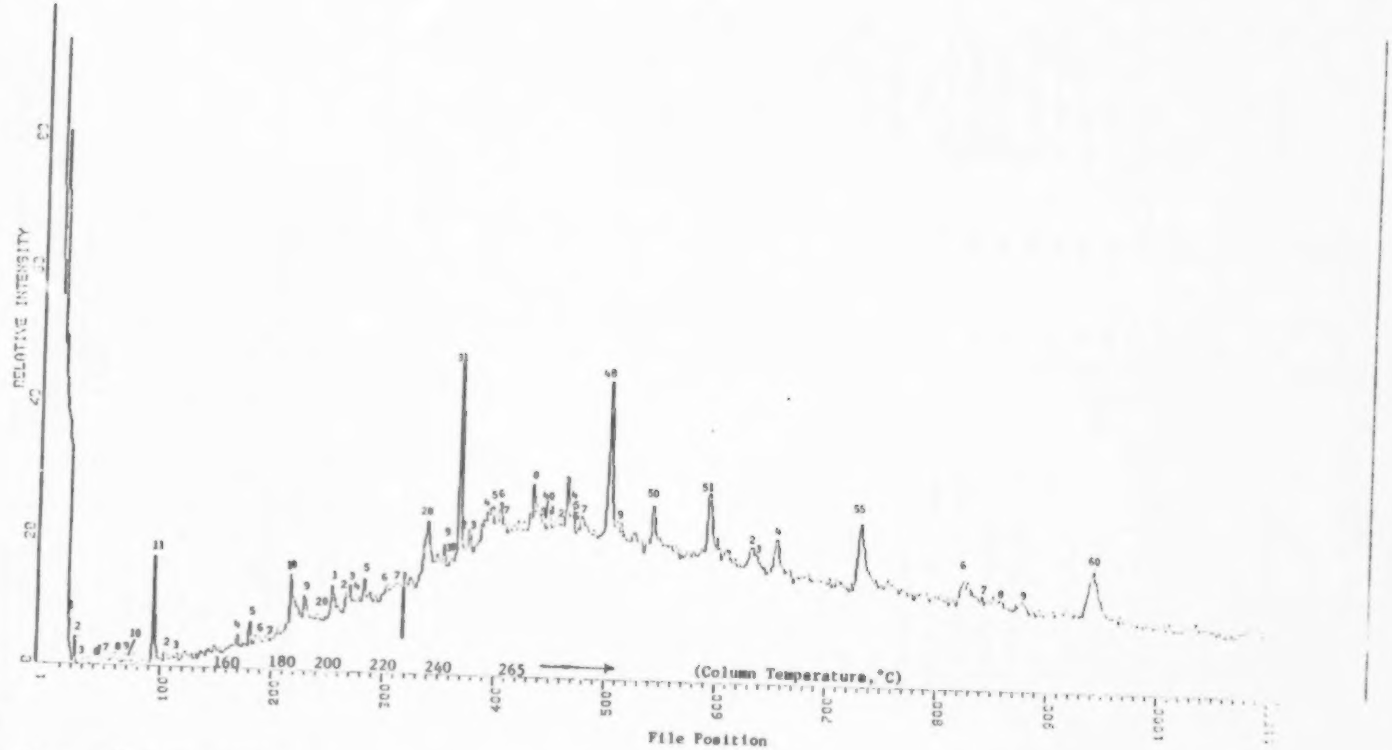


Figure F-2. Total ion current chromatogram of gc/ms/comp analysis of toluene extract of < 1.7 μ air particulate collected in Front Royal, VA (Trip 3, P1/L4).

Table F-2. COMPOUNDS IDENTIFIED IN TOLUENE EXTRACT OF <1.7μ FRACTION OF AIR PARTICULATE COLLECTED IN FRONT ROYAL, VA (TRIP 3, P1/L4).

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	100-112	toluene (solvent)
2	109	trimethylbenzene isomer
3	110.5	trimethylbenzene isomer
4	112	C_3H_7 benzene isomer
5	113	C_4H_9 benzene isomer
6	116	C_4H_9 and C_4H_7 benzene isomers
7	120	C_4H_9 benzene isomer (tent.)
8	122	C_4H_7 benzene isomer
9	127	naphthalene (tent.)
10	128	C_5H_9 benzene isomer
11	136-139	mixture of alkanes
12	141	phthalic anhydride
13	142	methylnaphthalene isomer
14	167	dibutylcresol isomer (bkg.)
15	172	unknown
16	173	dibutylcresol isomer (bkg.)
17	177	C_2 alkyl biphenyl (tent.)
18	187	Si cmpd. (bkg.)
19	191	4-hydroxy-3,5-dimethoxy-benzaldehyde
20	198.5	C_2 alkyl fluorene isomer (tent.)
21	201	$C_{15}H_{16}$ isomer[1]
22	206	unknown
23	207	$C_{14}H_{10}$ isomer[2]
24	208	phenothiazine (tent.)
25	212.5	xanthene (tent.)
26	220.5	naphthindenone isomer (tent.)
27	222	methyl $C_{14}H_{10}$ isomer
28	234.5	Si cmpd. (bkg.)
29	241	$C_{16}H_{10}$ isomer[3] (not pyrene)
30	244	$C_{16}H_{10}$ isomer[3] (not pyrene)
31	247	pyrene + pyrene-d_{10} (ext. std.)
32	248.5	$C_{18}H_{10}$ isomer[4]
33	251	unknown
34	258	methylpyrene isomer
35	260	$C_{17}H_{12}$ isomer[5] (tent.)
36	263	unknown
37	264	methylpyrene isomer
38	265	unknown
39	265	terphenyl isomer (tent.) + tri phenyl phosphate (bkg.)
40	265	terphenyl isomer (tent.)
41	265	$C_{18}H_{10}$ isomer[4]
42	265	$C_{18}H_{14}$ isomer[6]
43	265	$C_{18}H_{10}$ isomer[4]
44	265	$C_{18}H_{12}$ isomer[7]
45	265	$C_{18}H_{12}$ isomer[7]
46	265	$C_{18}H_{12}$ isomer[7]
47	265	benzanthrone
48	265	di-2-ethylhexylphthalate (bkg.)
49	265	$C_{19}H_{14}$ isomer[8] (tent.)
50	265	long-chain saturated hydrocarbon
51	265	$C_{20}H_{12}$ isomer[9]
52	265	$C_{20}H_{12}$ isomer[9]
53	265	$C_{20}H_{14}$ isomer[10]
54	265	$C_{20}H_{12}$ isomer[9]
55	265	long-chain saturated hydrocarbon
56	265	long-chain saturated hydrocarbon
57	265	$C_{22}H_{12}$ isomer[11]
58	265	$C_{22}H_{12}$ isomer[11]
59	265	$C_{22}H_{12}$ isomer[11]
60	265	$C_{22}H_{12}$ isomer[11]

Notes:

[1] $C_{15}H_{16}$ isomers include diphenylpropane isomers, ditolymethane isomers, and C_3 alkyl biphenyl isomers.

[2] $C_{14}H_{10}$ isomers include anthracene, phenanthrene, and biphenylacetylene.

[3] $C_{16}H_{10}$ isomers include pyrene, fluoranthene, and diphenyldiacetylene.

[4] $C_{18}H_{10}$ isomers include 1,10-benzfluoranthene and 3,4-cyclopentapyrene.

[5] $C_{17}H_{12}$ isomers include methylpyrene isomers and benzofluorene isomers.

[6] $C_{18}H_{14}$ isomers include terphenyl isomers, styrylnaphthalene isomers, diphenylbenzene isomers, and dihydrobenzathracene isomers.

[7] $C_{18}H_{12}$ isomers include chrysene, benzophenanthrene isomers, triphenylene, naphthacene, and benzanthracene isomers.

[8] $C_{19}H_{14}$ isomers include methyltriphenylene isomers, methylbenzanthracene isomers, methylchrysene isomers, and phenylfluorene.

[9] $C_{20}H_{12}$ isomers include perylenebenzpyrene isomers, and benzfluoranthene isomers.

[10] $C_{20}H_{14}$ isomers include binaphthyl isomers, anthracene benzyne adducts, 6,7-acechrysene, and triptycene.

[11] $C_{22}H_{12}$ isomers include 1,12-benzperylene, anthranthrene, and 2,3-o-phenylenepyrene.